

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. Mathematical Models and Methods in Applied Sciences, World Scientific Publishing, 2012, 22 (12), pp.1250038. <10.1142/S0218202512500388>. <inria-00533558v8>

HAL Id: inria-00533558

<https://hal.inria.fr/inria-00533558v8>

Submitted on 6 Aug 2011

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	5
3. Definitions and Notations	11
4. Proofs	11
4.1. Proof of Theorem 2.1	11
4.2. Proof of Theorem 2.2	14
4.3. Proof of Theorem 2.3	17
5. Examples	19
5.1. Examples for Theorem 2.2	19
5.2. Examples for Theorem 2.3	22
6. Auxiliary results	26
References	30

1. INTRODUCTION

The state of a quantum system is described by a positive, trace class operator D^ε , which evolves in time under the Heisenberg-von Neumann equation

$$(1.1) \quad \begin{aligned} i\varepsilon \frac{\partial}{\partial t} D^\varepsilon(t) &= \left[-\frac{\varepsilon^2}{2} \Delta + V, D^\varepsilon(t) \right], \\ D^\varepsilon(t=0) &= D_0^\varepsilon. \end{aligned}$$

Both the positivity and the trace of D^ε are preserved in time [20]; observables, also described by operators, can be measured against the state. For example, the value of observable \mathcal{G}^ε , associated with operator G^ε , at time t

is given by the trace $\mathcal{G}^\varepsilon(t) = \text{tr}(G^\varepsilon D^\varepsilon(t))$. The term *density matrix* is often used for a positive, trace-class operator.

The Heisenberg-von Neumann equation is closely related to the Schrödinger equation. By virtue of the singular value decomposition, the density matrix can be decomposed to a sum of *pure states*, i.e. rank-1 orthonormal projectors,

$$D^\varepsilon = \sum_m \lambda_m^\varepsilon |u_m^\varepsilon\rangle \langle \overline{u_m^\varepsilon}|$$

(the λ_m^ε 's are time-independent in the standard context of an external, time-independent potential, i.e. if V does not depend on D^ε , or t . Here we limit our scope to such problems). Then, each of the u_m^ε 's satisfies a problem of the form

$$(1.2) \quad \begin{aligned} i\varepsilon \frac{\partial}{\partial t} u_m^\varepsilon &= \left(-\frac{\varepsilon^2}{2} \Delta + V(x) \right) u_m^\varepsilon, \\ u_m^\varepsilon(t=0) &\in L^2. \end{aligned}$$

The small parameter ε is called Planck's constant, and when it tends to zero one expects the system to behave in a way approaching classical mechanics; i.e. motion under Newton's law in a force field with potential V . This is a singular asymptotic limit, and several techniques have been developed for its study; one is based on the Wigner transform (WT) [11, 12, 14].

The WT $W^\varepsilon(x, k, t)$ is defined as

$$(1.3) \quad W^\varepsilon(x, k, t) = W^\varepsilon[D^\varepsilon(t)](x, k) = \int_{y \in \mathbb{R}^n} e^{-2\pi i y k} K^\varepsilon(x + \varepsilon \frac{y}{2}, x - \varepsilon \frac{y}{2}, t) dy$$

where for each t , $K^\varepsilon(t)$ is the integral kernel of the operator $D^\varepsilon(t)$. The WT is also closely related to the Weyl symbol of D^ε , and the Weyl calculus of pseudodifferential operators in general, see e.g. [10] for more details in that direction. It evolves in time under the well-known Wigner equation,

$$(1.4) \quad \begin{aligned} \partial_t W^\varepsilon(x, k) + 2\pi k \cdot \partial_x W^\varepsilon(x, k) + \\ + \frac{2}{\varepsilon} \text{Re} \left[i \int e^{2\pi i S x} \widehat{V}(S) W^\varepsilon(x, k - \frac{\varepsilon S}{2}, t) dS \right] = 0, \end{aligned}$$

$$W^\varepsilon(t=0) = W_0^\varepsilon,$$

an equivalent reformulation of (1.1). In this context, it can be shown that observables can be measured by $\mathcal{G}^\varepsilon(t) = \int G_W^\varepsilon(x, k) W^\varepsilon(x, k) dx dk$, where $G_W^\varepsilon(x, k)$ is the Weyl symbol of the operator G^ε . (However this in general is not a Lebesgue integral, but only makes sense as a Cauchy PV one).

In the case of a *pure state*, $D^\varepsilon = |u^\varepsilon\rangle \langle \overline{u^\varepsilon}|$, the WT can be written as

$$(1.5) \quad W^\varepsilon(x, k, t) = \int_{y \in \mathbb{R}^n} e^{-2\pi i y k} u^\varepsilon(x + \varepsilon \frac{y}{2}, t) \overline{u^\varepsilon}(x - \varepsilon \frac{y}{2}, t) dy.$$

As a quadratic transform on an oscillating function u^ε , of small typical scale of oscillation ε , it has been widely used in signal processing, see e.g. [9] and a multitude of references therein for more on that direction.

Under appropriate conditions the WT allows for a very natural and compact description of the semiclassical limit. Indeed, it has a physically meaningful limit as ε tends to zero, while in general the operator D^ε itself does not. The limit (in an appropriate sense; see below for more precise statement and reference), is called the *Wigner measure*,

$$W^\varepsilon(t) \rightharpoonup W^0(t),$$

and is a probability measure that evolves in time under the Liouville equation of classical statistical mechanics

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

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

Observables are now described by bounded continuous functions, which can be measured against the classical state, $\mathcal{G}^0(t) = \int G^0(x, k) dW^0(t)$. The formal probabilistic interpretation e.g. for the expected position of a particle $\mathcal{X}(t) = \int x dW^0(t)$ should be intuitively clear.

Thus the correspondence between classical and quantum physics for the same system is highlighted in a very intuitive way, in terms of models that are, at least formally, similar and directly comparable. Convergence issues are not always painless or completely understood, as we will see in more detail. There is also the well-known caveat that $W^\varepsilon(t)$ is in general neither a measure of bounded total variation, nor non-negative e.g. as a distribution. Finally asking that the limit problem itself should be well-posed isn't always trivial.

Note at this point that considering initial data with

$$W^\varepsilon(0) \rightharpoonup \delta(x - x_0, k - k_0)$$

is particularly natural: they stand after all for classical particles with position x_0 and velocity k_0 .

It was shown in [14] (Théorème IV.1) that, under appropriate conditions on the initial data (which allow for practically all physically meaningful choices), as long as the potential is smooth enough, $V \in C^1$, the WT converges (in weak-* sense, and up to extraction of a subsequence) to a weak solution of the limit problem (1.6). It was immediately commented that, for $V \in C^1 \setminus C^{1,1}$, this does not yield an effective computation of the semiclassical limit in general, but only a partial description: even after the extraction of a subsequence (so that there is a unique $\lim_n W_0^{\varepsilon_n}$), in general there are several weak solutions for the Liouville equation that $W^{\varepsilon_n}(t)$ could converge towards (because the Liouville equation with $C^1 \setminus C^{1,1}$ potential and measure valued initial data has existence, but not uniqueness of weak solutions. This can be seen e.g. using the Peano Theorem). Therefore some kind of

selection principle would be needed to supplement the result, if we were to be able to identify the Wigner measure corresponding to our subsequence in ε of initial data. This, in a nutshell, is the context for the present work. Our goal is to understand better the mechanisms that may lead to loss of uniqueness, and develop tools which, at least in some cases, can resolve them.

We are particularly concerned with initial data that concentrate $W^\varepsilon(0) \rightharpoonup \delta(x-x_0, k-k_0)$, and our findings here apply, under appropriate assumptions, to such data. The main assumption (other than, essentially, $C^{1,\theta}$ potential regularity), is, roughly speaking, a non-concentration condition on the flow associated with the Liouville equation.

Before the statement of the present results, some reference to related works is warranted. The problem of extending semiclassical asymptotics to non-regular potentials (e.g. worse than $C^{1,1}$) has been studied by many authors – and for good reasons: some of the simplest, most natural systems (such as a gravitational or electrostatic force field) are described by potentials that are not C^1 , or C^1 . In most cases the conclusions make use of a particular form of singularity (e.g. Coulomb/piecewise smooth potential etc) as opposed to a general smoothness class [17, 13], and/or need some additional, non-trivial condition (non-concentration, non-interference etc) [17, 8]. Another type of results is for whole random populations of initial data [2] (which in particular can be even weaker than a result applying to “almost all” initial data; i.e. there might be no way to just choose “almost any” initial datum at $t = 0$ and keep track of it; the conclusions apply the population as a whole). Finally, it must be mentioned that in the study of the semiclassical limit in nonlinear problems (e.g. the Schrödinger-Poisson equation, a very natural problem), a lot remains to be understood. One of the main difficulties, comes precisely from the lack of regularity of the potential (which now depends on $D^\varepsilon(t)$), and the subsequent lack of well-posedness for the corresponding classical problem for measure-valued initial data; see e.g. [14, 16, 21].

More specifically, semiclassical limits with rough potentials were considered recently in [2] where the hypotheses on the potential are, roughly speaking, that it has a generic part with BV_{loc} gradient, plus possibly a *repulsive* Coulomb part. The setting involves a random population of initial data, and it is shown that the corresponding population of solutions at a later time tends weakly to the push-forward by the Liouville equation of a population of measures. The classical propagation problem for the random family of measures is shown to be well-posed by virtue of the Ambrosio-Di Perna-Lions theory [1, 7]. In [8] similar core ideas were used with deterministic mixed states. In that context, an averaging condition forbids initial data concentrating e.g. to a delta function in phase-space, a fact consistent with the weak limit strategy and the fact that the flow is not defined everywhere. The present work therefore concerns 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 point-supported measures.

The possible ill-posedness of the limit equation can originate not only from lack of smoothness of the potential, which we focused on for our discussion so far, but e.g. from working on a torus instead of Euclidean space [15].

Finally, let us present a concrete example. Already in [14], families of initial data were constructed so that their Wigner measures at later times oscillate between the several solutions of the Liouville equation. The one-dimensional case study used for that, was essentially equivalent to the following:

Consider 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 $|x| \geq 2$, and initial data such that $W_0^\varepsilon \rightharpoonup \delta(x - 0, k - 0)$. 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. $\forall t > 0$, or not at all; 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 is lost if we take the limit as usual in a straightforward way.

The first of our results deals explicitly with the case study from [14] mentioned earlier, to provide a clear illustration to the selection principle at work. 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 [14]: let

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

equipped with the norm

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

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 $W^\varepsilon(t)$ of (1.4) converges in weak-* sense in \mathcal{A}' to

$$(2.4) \quad W^0(t) = c_+ \delta(X^+(t), P^+(t)) + c_- \delta(X^-(t), P^-(t)),$$

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 [14], or Lemma 6.7).

In Remarque IV.3 of [14], 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. The present construction is different, and is not obtained through compactness arguments: there is no need of extraction of subsequence, and the scaling property is explicit (it is given by an implicit diagonal argument in a two scale sequence in [14]). The construction of [14] 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 non-concentration condition, which is relatively easy to check for other problems, whether the flow can be computed explicitly or not. (This may be increasingly important in high dimensions).

Let us also point out the similarity with the long-time behaviour around a regular separatrix, studied extensively in [18]. In the regular case, the quantum wavepacket leaves the fixed point in “infinite” (i.e. asymptotically long) time, as does the classical flow; here the classical flow leaves the fixed

point immediately, and this behaviour (under additional assumptions, of course) is preserved by the quantum system.

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

In the sequel we will consider potentials V that satisfy 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 approximate initial data $[W_0^\varepsilon] \in H^2(\mathbb{R}^{2n})$ such that*

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

and the solution of

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

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 $W^\varepsilon(t)$ of the solution of (1.4) satisfies, uniformly on $[0, T]$,

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

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

Remark: The non-concentration condition. It is helpful to discuss the motivation behind this type of assumption. Ideally, one would like the solution of the problem

$$\begin{aligned} \partial_t \rho + 2\pi k \cdot \partial_x \rho - \frac{1}{2\pi} \partial_x \tilde{V} \cdot \partial_k \rho &= 0, \\ \rho(t=0) &= W_0^\varepsilon \end{aligned}$$

to have H^2 regularity in the sense $\|\rho(t)\|_{H^2} \leq e^{Ct} \|W_0^\varepsilon\|_{H^2}$ for some C that is either ε -independent, or grows extremely slowly in ε . Of course, when working with low-regularity potentials, this is in general not possible. So one looks for a weaker version of regularity, which would still be sufficient here; it turns out that the property

$$\begin{aligned} \exists [W_0^\varepsilon] \in H^2(\mathbb{R}^{2n}), \quad \|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} &= o(\|W_0^\varepsilon\|_{L^2}) \text{ such that, if} \\ \partial_t \rho + 2\pi k \cdot \partial_x \rho - \frac{1}{2\pi} \partial_x \tilde{V} \cdot \partial_k \rho &= 0, \quad \rho(t=0) = [W_0^\varepsilon] \\ \text{then } \|\rho(t)\|_{H^2} &\text{ is not too large} \end{aligned}$$

is an acceptable surrogate.

We call this a non-concentration condition, because of one of the simplest ways to check it. Assume that there is a “small” set $S \subseteq \mathbb{R}^{2n}$, such that the derivatives of \tilde{V} up to order 3 outside S are “not too large” in ε . Now set $B = \bigcup_{t \in [0, T]} \phi_{-t}^\varepsilon(S)$, where ϕ_t^ε is the flow associated with the regularized

Liouville equation (2.8). B contains all the “dangerous” part of phase-space; away from B the original regularity requirement holds automatically. A “concentrating flow” could pull too big a part of phase-space through the original “small bad neighbourhood” S in time $t \in [0, T]$. On the other hand, a “repulsive singularity”, in general tends to push the flow away, thus keeping the pre-image of S small enough. The approximate initial data $[W_0^\varepsilon]$ can be then constructed by restricting the initial data on B^C .

Remark: Checking the assumptions for concrete problems. Concrete examples for which the assumptions (in particular the non-concentration condition) can be checked to hold, are examined in section 5. The techniques used can be easily extended to similar problems. It must be noted that the condition for Theorem 2.2 is seen to be satisfied for a generic selection of initial data, as long as the rate of concentration satisfies certain constraints (i.e. the profile that concentrates can be any function with a given regularity; see e.g. Lemmata 5.1, 5.2). In contrast, for the stronger Theorem 2.3 (see next Remark for the difference), in general we need to restrict the shape of the wavepacket with additional assumptions for the same problems; Lemmata 5.3, 5.4.

Remark: L^2 versus measures, and convergence. Theorem 2.2 is an L^2 asymptotic approximation result: two functions, of constant L^2 norm in time (also equal to one another and large in ε), are relatively close in L^2 . It is not, however, a convergence result, since in general neither function has a limit in L^2 . Ideally, we would like to conclude that, since they're

(relatively) close, both functions converge (in some appropriate sense) to the same limit, typically a (sum of) delta function(s). However, the (relative) L^2 approximation is not by itself sufficient to ensure that if e.g. $\rho_1^\varepsilon(t) \rightarrow \delta(x - x(t), k - k(t))$, then also $W^\varepsilon(t)$ goes to the same limit. Is there some additional information in the problem that we could use to come to that conclusion? Or is there a physical issue here, of L^2 norm really “missing” the solution? For example, is it really possible that in a problem with splitting (as in Theorem 2.1) the conclusion of Theorem 2.2 holds, in the limit ρ_1^ε “goes to the right”, but at the same time W^ε (or half its mass) “goes to the left”? This is a question that we cannot really answer at the moment. One possible way to go is by strengthening the non-concentration condition, and that is pursued in Theorem 2.3 below. This yields full control over the convergence (in an appropriate sense, see also Corollary 2.4), but at the cost of excluding many interesting, natural problems.

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*

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

$\|W_0^\varepsilon\|_{L^2} = o(\varepsilon^{-\kappa})$ (κ being the same as in Theorem 2.2), 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

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

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: L^2 versus measures, and convergence. If a generic “nice” function concentrates, $f^\varepsilon \rightarrow \delta(x, k)$, and $\|f^\varepsilon - [f^\varepsilon]\|_{L^1} = o(1)$, then it follows that $[f^\varepsilon] \rightarrow \delta(x, k)$ as well. In other words $\|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^1} = o(1)$ (which in general holds in the examples where Theorem 2.2 does) would be better suited to control concentration. We are forced however to use the much stronger $\|[W_0^\varepsilon] - W_0^\varepsilon\|_{L^2} = o(1)$ due to technical reasons, and in particular the fact

that the Wigner equation doesn't respect the L^1 norm in general (or the total variation of measures, or even the \mathcal{A}' norm away from the positive cone which also scale like L^1). The assumptions of Theorem 2.3 should be considered pessimistic, and probably can be relaxed. In any case, the precise convergence result is summarized in Corollary 2.4 below.

Remark: Size of the error. 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 $W^\varepsilon(t)$ 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.

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

if and only if

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

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 $\varepsilon \rightarrow 0$. 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.

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

FIGURE 1. In some cases, there is not enough information in $W^0(0)$ to determine $W^0(t)$, i.e. the Cauchy problem (1.6) is ill-posed.

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:

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

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. In this section we will show that Theorem 2.1 follows from Theorems 2.2, 2.3. The latter are proved in the next subsections.

Before getting into more detail, let us comment that λ as used in the statement of Theorem 2.1 is an effective upper bound. It is easily checked that if we replace λ by $\lambda' \leq \lambda$, $\frac{1}{\lambda'} = o(1)$, the Theorem still holds.

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

Now 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,

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

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 $\|\phi\|_{L^\infty} \leq \|\phi\|_{\mathcal{A}}$; recall that \mathcal{A} was defined in eq. (2.1)).

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

$$(4.5) \quad \begin{aligned} \dot{X}(t) &= 2\pi K(t), & \dot{K}(t) &= \frac{1+\theta}{2\pi} (X(t))^\theta, \\ X(0) &= CR, & K(0) &= |X(0)|^{\frac{1+\theta}{2}}, \end{aligned}$$

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: *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 readily follows that

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

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 (1.4) 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 ,

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

where $[W_0^\varepsilon]$ for now is simply assumed to exist (and have the properties found in the statement of Theorem 2.2. Such approximate initial data will be constructed, for concrete examples, in Section 5). Finally, 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:

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

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,

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

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

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

Asking that the remainder is small gives

$$\gamma > 1,$$

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

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

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

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

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

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

$$f(x, k, 0) = W_0^\varepsilon - [W_0^\varepsilon].$$

Using the Duhamel formula,
(4.20)

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

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 $b < 0$

$$\begin{aligned} (4.22) \quad & \left\| \int \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) \left(1 - \frac{\sin(\pi \varepsilon S \cdot K)}{\pi \varepsilon S \cdot K}\right) \pi S \cdot K dS \right\|_{L^2} \leq \\ & \leq C \varepsilon \left\| \int_{0 \leq |S| \leq 1} |\widehat{V}^\gamma(S)| \cdot |S|^2 |\widehat{\rho}_2^\varepsilon(X - S, K)| \cdot |K|^2 dS \right\|_{L^2} + \\ & + \varepsilon^{1+2b} \left\| \int_{1 < |S| \leq \varepsilon^b} \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) |K|^2 dS \right\|_{L^2} + \\ & + \left\| \int_{|S| > \varepsilon^b} \widehat{V}^\gamma(S) \widehat{\rho}_2^\varepsilon(X - S, K) |SK| dS \right\|_{L^2} \leq \\ & \leq C \left(\varepsilon^{1+2b} \|\widehat{V}(S) \min\{|S|^2, 1\}\|_{L^1} \|\rho_2^\varepsilon\|_{H^2} + \int_{|S| > \varepsilon^b} |\widehat{V}^\gamma(S)| |S| dS \|\rho_2^\varepsilon\|_{H^1} \right) \leq \\ & \leq C \left(\varepsilon^{1+2b} \|\widehat{V} \frac{S^2}{1+S^2}\|_{L^1} \|\rho_2^\varepsilon\|_{H^2} + \int_{\rho=\varepsilon^b}^{\infty} \rho^{-1-\theta} d\rho \|\rho_2^\varepsilon\|_{H^1} \right) = \\ & = C \left(\varepsilon^{1+2b} \|\rho_2^\varepsilon\|_{H^2} + \varepsilon^{-\theta b} \|\rho_2^\varepsilon\|_{H^1} \leq C(\varepsilon^{1+2b-\delta} + \varepsilon^{-\theta b - \delta}) \|W_0^\varepsilon\|_{L^2} \right) \end{aligned}$$

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

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

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), and $\|\rho_2^\varepsilon(t) - \rho_1^\varepsilon(t)\|_{L^2} = \|W_0^\varepsilon - [W_0^\varepsilon]\|_{L^2}$.

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

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

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 exists $R > 0$ such that $\|W^\varepsilon(t) - \rho_1^\varepsilon(t)\|_{\mathcal{A}'} < R$ for all $t \in [0, T]$.

Proof of the claim: Observe that

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

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 (1.2). The point is that the singular values are time-independent and,

especially for positive operators, are controlled by the trace:

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

We readily observe that

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

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, $\chi(z) = 1 \forall |z| < 1$, $\chi(z) = 0 \forall |z| > 2$, 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} [14]. 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; in that case it follows that $\|\phi_{M(\varepsilon)}\|_{L^2} \leq \frac{2^n \pi^{\frac{n}{2}}}{\sqrt{F(\varepsilon)^{n+1}}}$.

The proof is complete.

5. EXAMPLES

This section is devoted in understanding better the non-concentration properties that are in the heart of our main results. There are two versions; we isolate them below as “Property 1”, a condition to be checked for a given problem that is sufficient for Theorem 2.2 to apply to it, and the stronger “Property 2”, which is sufficient for Theorem 2.3 and its Corollary 2.4. Concrete examples of natural problems that satisfy either one or both of them are constructed; it must be noted that it’s rather easy to satisfy Property 1 to generic initial data and repulsive singularities. Asking that Property 2 holds is quite restrictive, and it seems that specially prepared initial data are needed for that.

We are only concerned here with examples that give rise to ill-posed classical problems. (Otherwise the existing theory for C^1 potentials has no problem to provide a complete description of the semiclassical limit).

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

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

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*

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

and the solution of

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

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.
- 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, for T small enough but independent from ε ,

$$\left(\bigcup_{t \in [0, T]} \text{supp} \rho_2^\varepsilon(t) \right) \cap \{|x| < R\} = \emptyset$$

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 in an $O(1)$ factor which we absorb in C below).

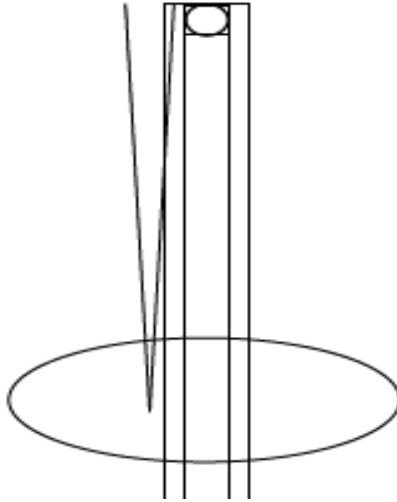


FIGURE 2. Any trajectory leaving the support of $[W_0^\varepsilon]$ has an initial velocity in a small cone around $k = (0, 1)$. If we were in free space, there wouldn't be enough space for sufficient movement in x_1 to reach $\{|x_1| < R\}$. Therefore the solution is the sum of two components, supported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

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

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

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

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

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

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

holds.

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

Property 2. *Given $V(x)$, W_0^ε 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

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

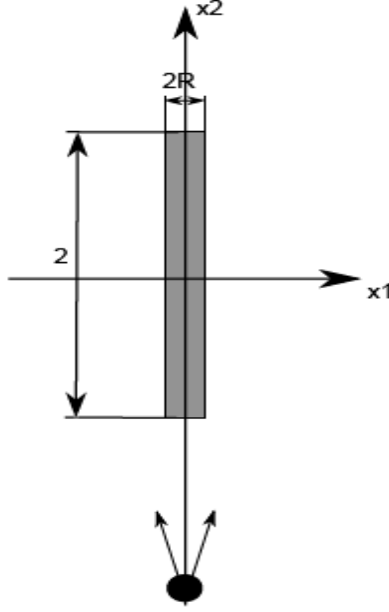


FIGURE 3. The construction of Lemma 5.1 holds, with obvious adjustments, to the example of Lemma 5.2.

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:

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

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.

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

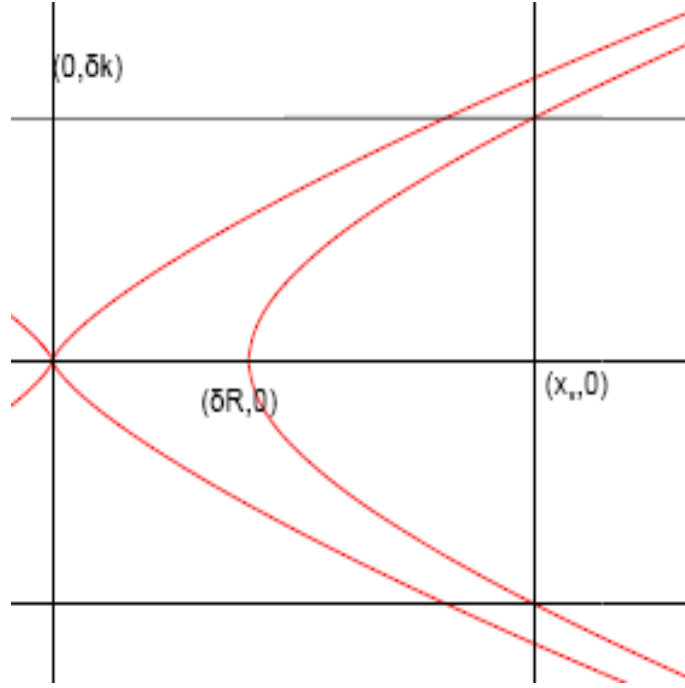


FIGURE 4. Schematic for Lemma 5.3; cutting off a strip in x , $\{|x| < x_*\}$, suffices to cut off the preimage of $\{|x| < R\}$

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 ,*

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

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

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

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

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

The proof is complete.

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

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

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

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

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 $\widetilde{V}_{eff}^\gamma$ in place of \widetilde{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 ($\widetilde{V}_{eff}^\gamma$ and R). *Let $V(x) = -|x|^{1+\theta}$. \widetilde{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

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

satisfies

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

while, of course,

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

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 \widetilde{V}^γ to $\{|x| < M\}$ without loss of generality,

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

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

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

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 [14]; we include here a brief mention for completeness:

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

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

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

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

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. Flandrin, “Time-frequency/Time-scale Analysis” (1998) Academic Press
- [10] G. Folland, “Harmonic Analysis in Phase-Space” (1989) Princeton University Press
- [11] 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.
- [12] P. Gérard, P. A. Markowich, N.J. Mauser & F. Poupaud, “Homogenization limits and Wigner transforms” (1997) *Comm. Pure Appl. Math.* **50** 323379
- [13] S. Keraani, “Wigner measures dynamics in a Coulomb potential” (2005) *J. Math. Phys.* **46** 063512
- [14] P.-L. Lions & T. Paul, “Sur les mesures de Wigner”, (1993) *Rev. Mat. Iberoamericana* **9** No. 3 553–618
- [15] F. Macia, “High-frequency propagation for the Schroedinger equation on the torus” (2010) *J. Funct. Anal.* **258** 933–955
- [16] P. A. Markowich & N. J. Mauser, “The classical limit of a self-consistent quantum Vlasov equation”, (1993) *Math. Mod. Meth. Appl. Sci.* **3** 109–124
- [17] L. Miller, “Refraction of high-frequency waves density by sharp interfaces and semiclassical measures at the boundary”, (2000) *J. Math. Pures Appl.* **79** (3) 227–269

- [18] 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).
- [19] M. Pulvirenti, “Semiclassical expansion of Wigner functions”, (2006) J. Mat. Phys. **47** 052103
- [20] M. Reed & B. Simon, “Functional Analysis (Methods of modern Mathematical Physics)” vol. II (1980), Academic Press
- [21] P. Zhang, Y. Zheng & N. J. Mauser, “The limit from the Schrödinger-Poisson to the Vlasov-Poisson equations with general data in one dimension” (2002) Comm. Pure Appl. Math. **55** 582-632

(A. Athanassoulis) DAMTP, UNIVERSITY OF CAMBRIDGE, WILBERFORCE ROAD, CAMBRIDGE CB3 0WA, UK

E-mail address: `a.athanassoulis@damtp.cam.ac.uk`

(T. Paul) CNRS AND CMLS, ÉCOLE POLYTECHNIQUE, 91128 PALAISEAU CEDEX, FRANCE

E-mail address: `thierry.paul@math.polytechnique.fr`