

Semiclassical limit for mixed states with singular and rough potentials

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Abstract

We consider the semiclassical limit for the Heisenberg-von Neumann equation with a potential which consists of the sum of a repulsive Coulomb potential, plus a Lipschitz potential whose gradient belongs to BV ; this assumption on the potential guarantees the well posedness of the Liouville equation in the space of bounded integrable solutions. We find sufficient conditions on the initial data to ensure that the quantum dynamics converges to the classical one. More precisely, we consider the Husimi functions of the solution of the Heisenberg-von Neumann equation, and under suitable assumptions on the initial data we prove that they converge, as $\varepsilon \rightarrow 0$, to the unique bounded solution of the Liouville equation (locally uniformly in time).

1 Introduction

The aim of this paper is to study the semiclassical limit for the Heisenberg-von Neumann (quantum Liouville) equation:

$$\begin{cases} i\varepsilon\partial_t\tilde{\rho}_t^\varepsilon = [H_\varepsilon, \tilde{\rho}_t^\varepsilon], \\ \tilde{\rho}_0^\varepsilon = \tilde{\rho}_{0,\varepsilon}, \end{cases} \quad (1.1)$$

$\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon>0}$ being a family of uniformly bounded (with respect to ε), positive, trace class operators, and with $H_\varepsilon = -\frac{\varepsilon^2}{2}\Delta + U$.

When $\tilde{\rho}_{0,\varepsilon}$ is the orthogonal projector onto $\psi_{0,\varepsilon} \in L^2(\mathbb{R}^n)$, (1.1) is equivalent (up to a global phase) to the Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t\psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi_t^\varepsilon + U\psi_t^\varepsilon = H_\varepsilon\psi_t^\varepsilon, \\ \psi_0^\varepsilon = \psi_{0,\varepsilon} \in L^2(\mathbb{R}^n), \end{cases} \quad (1.2)$$

We recall that the Wigner transform $W_\varepsilon\psi$ of a function $\psi \in L^2(\mathbb{R}^n)$ is defined as

$$W_\varepsilon\psi(x, p) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \psi\left(x + \frac{\varepsilon}{2}y\right) \overline{\psi\left(x - \frac{\varepsilon}{2}y\right)} e^{-ipy} dy,$$

and the one of a density matrix $\tilde{\rho}$ is defined as

$$W_\varepsilon\rho(x, p) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \rho\left(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y\right) e^{-ipy} dy, \quad (1.3)$$

where $\rho(x, x')$ denotes the integral kernel associated to the operator $\tilde{\rho}$.

The weak limit of the Wigner function of the solution of (1.2) or (1.1) has been studied in many articles (e.g. [16, 14, 15], and more recently in strong topology in [6, 7]). More precisely, it is well-known that the limit dynamics of the Schrödinger equation is related to the Liouville equation

$$\partial_t \mu + p \cdot \nabla_x \mu - \nabla U(x) \cdot \nabla_p \mu = 0, \quad (1.4)$$

and, roughly speaking, the above results state that:

(A) If U is of class C^2 and there exists a sequence $\varepsilon_k \rightarrow 0$ such that $W_{\varepsilon_k} \rho_{0, \varepsilon_k}$ converges in the sense of distributions to some (nonnegative) measure μ_0 , then the Wigner functions at any other time $W_{\varepsilon_k} \rho_t^{\varepsilon_k}$ converge to $(\Phi_t)_\# \mu_0$ (the convergence is again in the sense of distributions), where Φ_t is the (unique) flow map associated to the Hamiltonian system

$$\begin{cases} \dot{x} = p, \\ \dot{p} = -\nabla U(x) \end{cases} \quad (1.5)$$

so that $\mu_t := (\Phi_t)_\# \mu_0$ is the unique solution to (1.4) (here and in the sequel, $\#$ denotes the push-forward, so that $\mu_t(A) = \mu_0(\Phi_t^{-1}(A))$ for all $A \subset \mathbb{R}^{2n}$ Borel).

(B) If U is of class C^1 and there exists a sequence $\varepsilon_k \rightarrow 0$ such that the initial Wigner function $W_{\varepsilon_k} \rho_{0, \varepsilon_k}$ converges in the sense of distributions to some (nonnegative) measure μ_0 , then the curve $t \mapsto W_{\varepsilon_k} \rho_t^{\varepsilon_k}$, up to a subsequence, converges in the sense of distributions to some curve of (nonnegative) measure $t \mapsto \mu_t$, and μ_t solves (1.4). Of course, since the Hamilton system (1.5) may not have a unique solution, the limit μ_t is no longer uniquely determined and it can depend on the subsequence.

(C) In [5] it has been proved that (B) holds even in presence of Coulomb singularities, namely $U = U_s + U_b$, where U_s is the repulsive Coulomb potential and U_b is C^1 .

(D) In a recent paper [1], this literature has been improved in two directions:

- (i) By lowering the regularity assumptions on the potential in order to get convergence results for a more general class of potentials: roughly speaking, the potential U_b is bounded, locally Lipschitz, and $\nabla U_b \in BV_{\text{loc}}$ (plus some conditions about its growth at infinity);
- (ii) Remove the passing to a subsequence argument, due to compactness, used in most of the available proofs where one is unable to uniquely identify the limit.

The price to pay for the lack of regularity of the potential is that it is not possible to consider pure states as initial data because the Wigner function of pure states can concentrate at a point, a possibility which might actually enter in conflict with the fact that the underlying flow is not uniquely defined everywhere in presence of non-smooth potentials.

In order to avoid this problem, in the same spirit of the theory of flows developed by Di Perna and Lions, in [1] it is considered a family of Schrödinger equation

$$\begin{cases} i\varepsilon \partial_t \psi_{t,w}^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi_{t,w}^\varepsilon + U \psi_{t,w}^\varepsilon = H_\varepsilon \psi_{t,w}^\varepsilon, \\ \psi_{0,w}^\varepsilon = \psi_{0,\varepsilon,w} \in L^2(\mathbb{R}^n), \end{cases} \quad (1.6)$$

indexed by a random parameter $w \in W$ running in a probability space $(W, \mathcal{F}, \mathbb{P})$, and the family of the solutions of (1.6) is analyzed as a whole. The result in [1] is the following: if the family of initial data satisfies the the “no-concentration in mean” assumption

$$\frac{1}{\varepsilon^n} \int_W |\psi_{0,\varepsilon,w}\rangle\langle\psi_{0,\varepsilon,w}| d\mathbb{P}(w) \leq C \text{Id} \quad (1.7)$$

then

$$\lim_{\varepsilon \rightarrow 0} \int_W \sup_{t \in [0, T]} d_{\mathcal{D}} \left(\tilde{W}_\varepsilon \psi_{t,w}^\varepsilon, \boldsymbol{\mu}(t, \mu_w) \right) d\mathbb{P}(w) = 0, \quad \forall T > 0. \quad (1.8)$$

Here $d_{\mathcal{D}}$ is any bounded distance inducing the weak topology in $\mathcal{D}(\mathbb{R}^{2n})$, $\tilde{W}_\varepsilon \psi_{t,w}^\varepsilon$ is the Husimi transform of $\psi_{t,w}^\varepsilon$ defined in (1.9), and $\boldsymbol{\mu}(t, \mu_w)$ is a “ \mathbb{P} -a.s. uniquely identified” limit such that $t \mapsto \boldsymbol{\mu}(t, \mu_w)$ solves (1.4) with $\boldsymbol{\mu}(0, \mu_w) := \lim_\varepsilon \tilde{W}_\varepsilon \psi_{0,\varepsilon,w}$.

The idea behind this result it to use the Ambrosio-Bouchut-DiPerna-Lions’ theory of flows for ODEs with BV vector fields: more precisely, the uniqueness of solutions to (1.4) in the space $L^\infty_+([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$ (see Paragraph 2.2 below) is exploited to obtain a family of solutions of (1.4) $\{\boldsymbol{\mu}(t, \mu_w)\}_{w \in W}$ which is “unique almost surely” and to which the Husimi measures converge with probability one (see [1] for more details).

In the present paper we want to extend some ideas contained in [1] in order to prove convergence results for the Heisenberg-von Neumann equation, under the same regularity assumptions on the potential U as in [1]. More precisely, as we said above, the idea in [1] was to consider a random family of Schrödinger equations and consider a no-concentration in mean assumption on the initial data. This reminds the theory of density operators, and it is natural to wonder whether the above strategy may be used to prove well-posedness for the Heisenberg Von-Neumann equation under a “no-concentration assumption” on the initial data (now without the need to average the initial data with respect to a random parameter, as a density matrix is already an average of pure states). Let us point out that the result for general density matrices cannot be recovered as a corollary of [1]: indeed, in [1] the authors consider averages of pure states with respect to a *fixed* probability measure which does not depend on ε , while, using the spectral decomposition, a density matrix of trace class is an average of pure states with respect to a measure which depends on the matrix itself.

As described below, we will show that, for general bounded and globally Lipschitz potential associated to locally *BV* vector fields (in addition to some Coulomb part), the Wigner measure of the solution at any time is the push-forward of the initial one by the Ambrosio-Bouchut-DiPerna-Lions flow [10, 8, 2]. An important difference with respect to [1] is that here we can avoid using the theory of flows in the space of probability measures developed in [1, 4], needing only the theory of flows in \mathbb{R}^{2n} . So, although some non-trivial improvements with respect to [1] are needed, avoiding the theory of flows in the space of probability measures has the advantage of considerably simplifying the presentation, making the argument more accessible to a broader audience.

As explained before the price to pay for the lack of regularity of the potential will be to have some no-concentration assumptions on the initial data which forbids the possibility of considering pure states. Let us mention however that, with extra assumptions on the potential (but still

allowing the possibility of not having uniqueness of a classical flow), it is possible to consider concentrating initial Wigner functions, giving rise to atomic measures whose evolution follows the “multicharacteristics” of the flow (see [7]).

Our method will use extensively the Husimi transforms $\psi \mapsto \tilde{W}_\varepsilon \psi$ and $\rho \mapsto \tilde{W}_\varepsilon \rho$, which we recall are defined in terms of convolution of the Wigner transform with the $2n$ -dimensional Gaussian kernel with variance $\varepsilon/2$:

$$\tilde{W}_\varepsilon \psi := (W_\varepsilon \psi) * G_\varepsilon^{(2n)}, \quad \tilde{W}_\varepsilon \rho := (W_\varepsilon \rho) * G_\varepsilon^{(2n)}, \quad G_\varepsilon^{(2n)}(x, p) := \frac{e^{-(|x|^2 + |p|^2)/\varepsilon}}{(\pi\varepsilon)^n} = G_\varepsilon^{(n)}(x)G_\varepsilon^{(n)}(p). \quad (1.9)$$

Of course, the asymptotic behaviour of the Wigner and Husimi transform is the same in the limit $\varepsilon \rightarrow 0$. However, one of the main advantages of the Husimi transform is that it is nonnegative (see Appendix).

Let us observe that, thanks to (A.8), the L^∞ -norm of $\tilde{W}_\varepsilon \psi$ can be estimated using the Cauchy-Schwarz inequality:

$$\tilde{W}_\varepsilon \psi(x, p) \leq \frac{1}{\varepsilon^n} \|\psi\|_{L^2}^2 \|\phi_{x,p}^\varepsilon\|_{L^2}^2 = \frac{\|\psi\|_{L^2}^2}{\varepsilon^n}.$$

However, this estimate blows up as $\varepsilon \rightarrow 0$. On the other hand we will prove that, by averaging the initial condition with respect to translations, we can get a uniform estimate as $\varepsilon \rightarrow 0$ (Section 3.2). This gives us, for instance, an important family of initial data to which our result and the ones in [1] apply (see also the other examples in Section 3).

2 The main results

2.1 Setting

We are concerned with the derivation of classical mechanics from quantum mechanics, corresponding to the study of the asymptotic behaviour of solutions $\tilde{\rho}_t^\varepsilon$ to the Heisenberg-von Neumann equation

$$\begin{cases} i\varepsilon \partial_t \tilde{\rho}_t^\varepsilon = [H_\varepsilon, \tilde{\rho}_t^\varepsilon] \\ \tilde{\rho}_0^\varepsilon = \tilde{\rho}_{0,\varepsilon}, \end{cases} \quad (2.1)$$

as $\varepsilon \rightarrow 0$, where $H_\varepsilon = -\frac{\varepsilon^2}{2} \Delta + U$, and $U : \mathbb{R}^n \rightarrow \mathbb{R}$ is of the form $U_b + U_s$ on \mathbb{R}^n , where U_s is a repulsive Coulomb potential

$$U_s(x) = \sum_{1 \leq i < j \leq M} \frac{Z_i Z_j}{|x_i - x_j|}, \quad M \leq n/3, \quad x = (x_1, \dots, x_M, \bar{x}) \in (\mathbb{R}^3)^M \times \mathbb{R}^{n-3M}, \quad Z_i > 0,$$

U_b is globally bounded, locally Lipschitz, $\nabla U_b \in BV_{\text{loc}}(\mathbb{R}^n; \mathbb{R}^n)$, and

$$\text{ess sup}_{x \in \mathbb{R}^n} \frac{|\nabla U_b(x)|}{1 + |x|} < +\infty.$$

The potential $U = U_s + U_b$ satisfies the standard Kato conditions and thus the operator H_ε is selfadjoint on $L^2(\mathbb{R}^n)$ with domain $H^2(\mathbb{R}^n)$. The formal solution of (1.2) is $\tilde{\rho}_t^\varepsilon$, where

$$\tilde{\rho}_t^\varepsilon := e^{-itH_\varepsilon/\varepsilon} \tilde{\rho}_{0,\varepsilon} e^{itH_\varepsilon/\varepsilon}$$

and its kernel is ρ_t^ε . Moreover, as shown for instance in [16], $W_\varepsilon \rho_t^\varepsilon$ solves in the sense of distributions the equation

$$\partial_t W_\varepsilon \rho_t^\varepsilon + p \cdot \nabla_x W_\varepsilon \rho_t^\varepsilon = \mathcal{E}_\varepsilon(U, \rho_t^\varepsilon), \quad (2.2)$$

where $\mathcal{E}_\varepsilon(U, \rho)$ is given by

$$\mathcal{E}_\varepsilon(U, \rho)(x, p) := -\frac{i}{(2\pi)^n} \int_{\mathbb{R}^n} \left[\frac{U(x + \frac{\varepsilon}{2}y) - U(x - \frac{\varepsilon}{2}y)}{\varepsilon} \right] \rho(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) e^{-ipy} dy. \quad (2.3)$$

Adding and subtracting $\nabla U(x) \cdot y$ in the term in square brackets and using $ye^{-ipy} = i\nabla_p e^{-ipy}$, an integration by parts gives $\mathcal{E}_\varepsilon(U, \rho) = \nabla U(x) \cdot \nabla_p W_\varepsilon \rho + \mathcal{E}'_\varepsilon(U, \rho)$, where $\mathcal{E}'_\varepsilon(U, \rho)$ is given by

$$\mathcal{E}'_\varepsilon(U, \rho)(x, p) := -\frac{i}{(2\pi)^n} \int_{\mathbb{R}^n} \left[\frac{U(x + \frac{\varepsilon}{2}y) - U(x - \frac{\varepsilon}{2}y)}{\varepsilon} - \nabla U(x) \cdot y \right] \rho(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) e^{-ipy} dy. \quad (2.4)$$

Let $\mathbf{b} : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ be the autonomous divergence-free vector field $\mathbf{b}(x, p) := (p, -\nabla U(x))$. Then, by the discussion above, $W_\varepsilon \rho_t^\varepsilon$ solves the Liouville equation associated to \mathbf{b} with an error term:

$$\partial_t W_\varepsilon \rho_t^\varepsilon + \mathbf{b} \cdot \nabla W_\varepsilon \rho_t^\varepsilon = \mathcal{E}'_\varepsilon(U, \rho_t^\varepsilon). \quad (2.5)$$

On the other hand, thanks to (2.2), it is not difficult to prove that $\tilde{W}_\varepsilon \rho_t^\varepsilon$ solves in the sense of distributions the equation

$$\partial_t \tilde{W}_\varepsilon \rho_t^\varepsilon + p \cdot \nabla_x \tilde{W}_\varepsilon \rho_t^\varepsilon = \mathcal{E}_\varepsilon(U, \rho_t^\varepsilon) * G_\varepsilon^{(2n)} - \sqrt{\varepsilon} \nabla_x \cdot [W_\varepsilon \rho_t^\varepsilon * \bar{G}_\varepsilon^{(2n)}], \quad (2.6)$$

where

$$\bar{G}_\varepsilon^{(2n)}(y, q) := \frac{q}{\sqrt{\varepsilon}} G_\varepsilon^{(2n)}(y, q). \quad (2.7)$$

Since $W_\varepsilon \rho_t^\varepsilon$ and $\tilde{W}_\varepsilon \rho_t^\varepsilon$ have the same limit points as $\varepsilon \rightarrow 0$, the heuristic idea is that in the limit $\varepsilon \rightarrow 0$ all error terms should disappear, and we should be left with the Liouville equation (which describes the classical dynamics)

$$\partial_t \omega_t + \mathbf{b} \cdot \nabla \omega_t = 0 \quad \text{on } \mathbb{R}^{2n}.$$

2.2 Preliminary results on the Liouville equations

Under the above assumptions on U one cannot hope for a general uniqueness result in the space of measures for the Liouville equation, as this would be equivalent to uniqueness for the ODE with vector field \mathbf{b} (see for instance [3]). On the other hand, as shown in [1, Theorem 6.1], the equation

$$\begin{cases} \partial_t \omega_t + \mathbf{b} \cdot \nabla \omega_t = 0 \\ \omega_0 = \bar{\omega} \in L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}) \text{ and nonnegative,} \end{cases} \quad (2.8)$$

has existence and uniqueness in the space $L_+^\infty([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$. This means that there exist a unique $\mathscr{W} : [0, T] \rightarrow L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$, nonnegative and such that $\text{ess sup}_{t \in [0, T]} \|\mathscr{W}_t\|_{L^1(\mathbb{R}^{2n})} + \|\mathscr{W}_t\|_{L^\infty(\mathbb{R}^{2n})} < +\infty$, that solves (2.8) in the sense of distributions on $[0, T] \times \mathbb{R}^{2n}$.

One may wonder whether, in this general setting, solutions to the transport equation can still be described using the theory of characteristics. Even if in this case one cannot solve uniquely the ODE, one can still prove that there exists a unique flow map in the ‘‘Ambrosio-DiPerna-Lions sense’’. Let us recall the definition of *Regular Lagrangian Flow* (in short RLF) in the sense of Ambrosio-DiPerna-Lions (here and in the sequel, \mathcal{L}^n denotes the Lebesgue measure on \mathbb{R}^n):

We say that a (continuous) family of maps $\Phi_t : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$, $t \geq 0$, is a RLF associated to (1.5) if:

- Φ_0 is the identity map.
- For \mathcal{L}^{2n} -a.e. (x, p) , $t \mapsto \Phi_t(x, p)$ is an absolutely continuous curve solving (1.5).
- For every $T > 0$ there exists a constant C_T such that $(\Phi_t)_\# \mathcal{L}^{2n} \leq C_T \mathcal{L}^{2n}$ for all $t \in [0, T]$.

Observe that, since ∇U is not Lipschitz, a priori the ODE (1.5) could have more than one solution for some initial condition. However, the approach via RLFs allows to get rid of this problem by looking at solutions to (1.5) as a whole, and under suitable assumptions on U the RLF associated to (1.5) exists, and it is unique in the following sense: assume that Φ^1 and Φ^2 are two RLFs. Then, for \mathcal{L}^{2n} -a.e. (x, p) , $\Phi_t^1(x, p) = \Phi_t^2(x, p)$ for all $t \in [0, +\infty)$. In particular, as shown in [1, Section 6], the unique solution to (2.8) is given by

$$\omega_t \mathcal{L}^{2n} = (\Phi_t)_\# (\bar{\omega} \mathcal{L}^{2n}). \quad (2.9)$$

Hence, the idea is that, if we can ensure that any limit point of the Husimi transforms $\tilde{W}_\varepsilon \rho_t^\varepsilon$ gives rise to a curve of measure belonging to $L_+^\infty([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$, by the aforementioned result we would deduce that the limit is unique (once the limit initial datum is fixed), and moreover it is transported by the unique RLF. In order to get such a result we need to make some assumptions on the initial data.

2.3 Assumptions on the initial data and main theorem

Let $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$ be a family of initial data which satisfy

$$\tilde{\rho}_{0,\varepsilon} = \tilde{\rho}_{0,\varepsilon}^*, \quad \tilde{\rho}_{0,\varepsilon} \geq 0, \quad \text{and} \quad \text{tr}(\tilde{\rho}_{0,\varepsilon}) = 1 \quad \forall \varepsilon \in (0,1).$$

Let

$$\tilde{\rho}_{0,\varepsilon} = \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)}, \cdot \rangle \phi_j^{(\varepsilon)}$$

be the spectral decomposition of $\tilde{\rho}_{0,\varepsilon}$, and denote by $\rho_{0,\varepsilon}$ its integral kernel.

We assume:

$$\sup_{\varepsilon \in (0,1)} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_j^{(\varepsilon)}\|^2 = c_1 < +\infty, \quad (2.10)$$

$$\frac{1}{\varepsilon^n} \tilde{\rho}_{0,\varepsilon} \leq C \text{Id}, \quad (2.11)$$

$$\lim_{R \rightarrow +\infty} \sup_{\varepsilon \in (0,1)} \int_{\mathbb{R}^n \setminus B_R^{(n)}} \rho_{0,\varepsilon}(x, x) dx = 0, \quad (2.12)$$

and

$$\lim_{R \rightarrow +\infty} \sup_{\varepsilon \in (0,1)} \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n \setminus B_R^{(n)}} \mathcal{F} \rho_{0,\varepsilon} \left(\frac{p}{\varepsilon}, \frac{p}{\varepsilon} \right) dp = 0, \quad (2.13)$$

where $B_R^{(n)}$ is the ball of radius R in \mathbb{R}^n and \mathcal{F} is the Fourier transform on \mathbb{R}^{2n} , see (A.5). Conditions (2.12) and (2.13) are equivalent to asking that the family of probability measure $\{\tilde{W}_\varepsilon \rho_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$ is tight (see Appendix). By Prokhorov's Theorem, this is equivalent to the compactness of $\{\tilde{W}_\varepsilon \rho_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$ with respect to the weak topology of probability measures (i.e., in the duality with $C_b(\mathbb{R}^{2n})$, the space of bounded continuous functions). Hence, up to extracting a subsequence, assumptions (2.12) together with (2.13) is equivalent to the existence of a probability density $\bar{\omega}$ such that

$$w - \lim_{\varepsilon \rightarrow 0} \tilde{W}_\varepsilon \rho_{0,\varepsilon} \mathcal{L}^{2n} = \bar{\omega} \mathcal{L}^{2n} \in \mathcal{P}(\mathbb{R}^{2n}), \quad (2.14)$$

where $\mathcal{P}(\mathbb{R}^{2n})$ denotes the space of probability measures on \mathbb{R}^{2n} . In order to avoid a tedious notation which would result by working with a subsequence ε_k , we will assume that (2.14) holds along the whole sequence $\varepsilon \rightarrow 0$, keeping in mind that all the arguments could be repeated with an arbitrary subsequence.

Let us observe that condition (2.10) is slightly weaker than $\sup_{\varepsilon \in (0,1)} \text{tr}(H_\varepsilon^2 \tilde{\rho}_{0,\varepsilon}) < +\infty$: indeed, although they are formally the same, to give a meaning to the latter we need the operator $H_\varepsilon^2 \tilde{\rho}_t^\varepsilon$ to make sense (at least on a core). Concerning assumption (2.14), we observe that the hypothesis $\text{tr}(\tilde{\rho}_{0,\varepsilon}) = 1$ implies that $\tilde{W}_\varepsilon \rho_{0,\varepsilon} \in \mathcal{P}(\mathbb{R}^{2n})$ (see Appendix).

To express in a better and cleaner way the fact that the convergence is uniform in time, we denote by $d_{\mathcal{P}}$ any bounded distance inducing the weak topology in $\mathcal{P}(\mathbb{R}^{2n})$. Recall also that Φ_t denotes the unique RLF associated to $\mathbf{b}(x, p) = (p, -\nabla U(x))$, so that $(\Phi_t)_\#(\bar{\omega} \mathcal{L}^{2n})$ is the unique nonnegative solution of (2.8) in $L_+^\infty([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$.

Theorem 2.1. *Let U be as in Section 2.1. Under the assumptions (2.10), (2.11) and (2.14)*

$$\lim_{\varepsilon \rightarrow 0} \sup_{[0, T]} d_{\mathcal{P}} \left(\tilde{W}_\varepsilon \rho_t^\varepsilon \mathcal{L}^{2n}, (\Phi_t)_\#(\bar{\omega} \mathcal{L}^{2n}) \right) = 0. \quad (2.15)$$

Moreover, if we define $\mathcal{W}_t \mathcal{L}^{2n} = (\Phi_t)_\#(\bar{\omega} \mathcal{L}^{2n})$, for every smooth function $\varphi \in C_c^\infty(\mathbb{R}^{2n})$ the map $t \mapsto \int_{\mathbb{R}^{2n}} \varphi \mathcal{W}_t dx dp$ is continuously differentiable.

The rest of the paper will be concerned with the proof of Theorem 2.1. However, before proceeding with the proof, we first provide some example and sufficient conditions for our result to apply.

3 Examples

We will give three types of examples of density matrices satisfying the assumptions of the preceding section, so that Theorem 2.1 applies.

3.1 Average of an orthonormal basis

For simplicity, we set up our first example in the one-dimensional case. In particular, there is no Coulomb interaction (that is, $U = U_b$), since by assumption Coulomb interactions are three-dimensional. We leave to the interested reader the extension to arbitrary dimension (the only difference in the case $U_s \neq 0$ appears when checking assumption (2.10)).

Let us consider the orthonormal basis of $L^2(\mathbb{R})$ given by the (semiclassical) Hermite functions

$$\psi_j^{(\varepsilon)}(x) = \frac{e^{-x^2/2\varepsilon}}{\sqrt{2^j j! (\pi\varepsilon)^{1/4}}} H_j \left(\frac{x}{\sqrt{\varepsilon}} \right), \quad j \in \mathbb{N},$$

where H_j 's are the Hermite polynomials, i.e.

$$H_j(x) = (-1)^j e^{x^2} \frac{d^j}{dx^j} e^{-x^2}.$$

The following holds:

Proposition 3.1. *Let $\{\mu_j^{(\varepsilon)}\}_{j \in \mathbb{N}}$ be a sequence of positive numbers, and consider the density matrix ρ_ε given by*

$$\rho_\varepsilon = \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \langle \psi_j^{(\varepsilon)}, \cdot \rangle \psi_j^{(\varepsilon)}.$$

Assume that

- $0 \leq \mu_j^{(\varepsilon)} \leq C\varepsilon$, $\sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} = 1$;
- $\varepsilon^2 \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} j^2 \leq C < +\infty$;
- $w - \lim_{\varepsilon \rightarrow 0} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \delta(x^2 + p^2 - j\varepsilon) = \bar{\omega} \mathcal{L}^2 \in \mathcal{P}(\mathbb{R}^2)$.

Then (2.10), (2.11), and (2.14) hold.

Proof. The first assumption is equivalent to (2.11) and the trace-one condition.

Concerning (2.10), using the well-know fact that

$$\varepsilon \frac{d}{dx} \psi_j^{(\varepsilon)} = \sqrt{\frac{\varepsilon}{2}} \left(\sqrt{j} \psi_{j-1}^{(\varepsilon)} - \sqrt{j+1} \psi_{j+1}^{(\varepsilon)} \right),$$

by a simple calculation it follows that

$$\begin{aligned} H_\varepsilon \psi_j^{(\varepsilon)} &= -\frac{\varepsilon^2}{2} \frac{d^2}{dx^2} \psi_j^{(\varepsilon)} + U_b \psi_j^{(\varepsilon)} \\ &= -\frac{\varepsilon}{4} \left(\sqrt{j(j-1)} \psi_{j-2}^{(\varepsilon)} - (2j+1) \psi_j^{(\varepsilon)} + \sqrt{(j+1)(j+2)} \psi_{j+2}^{(\varepsilon)} \right) + U_b \psi_j^{(\varepsilon)}. \end{aligned}$$

Hence

$$\begin{aligned} \|H_\varepsilon \psi_j^{(\varepsilon)}\|^2 &\leq \left[\frac{\varepsilon}{4} \left(\sqrt{j(j-1)} + (2j+1) + \sqrt{(j+1)(j+2)} \right) + \|U_b\|_\infty \right]^2 \\ &\leq C(1 + \varepsilon^2 j^2), \end{aligned}$$

and (2.10) follows from the first two assumptions.

Finally, the third assumption implies (2.14) by noticing that

$$w - \lim_{\varepsilon \rightarrow 0, j \rightarrow \infty, j\varepsilon \rightarrow a} \tilde{W}_\varepsilon \psi_j^{(\varepsilon)} = \delta(x^2 + p^2 - a) \quad \forall a \geq 0$$

(see, for instance, [16, Exemple III.6]). □

3.2 Töplitz case

Let $\phi \in H^2(\mathbb{R}^n; \mathbb{C})$ with $\int_{\mathbb{R}^n} |\phi(x)|^2 dx = 1$. Given $\varepsilon, \varsigma > 0$, for any $w, q \in \mathbb{R}^n$ let $\psi_{w,q}^\varepsilon$ be defined by

$$\psi_{w,q}^\varepsilon(x) := \frac{1}{\varsigma^{n/2}} \phi\left(\frac{x-q}{\varsigma}\right) e^{i\frac{w \cdot x}{\varepsilon}}.$$

Then, using Plancherel theorem, one can easily check that the identity

$$\frac{1}{\varepsilon^n} \int_{\mathbb{R}^{2n}} |\psi_{w,q}^\varepsilon\rangle \langle \psi_{w,q}^\varepsilon| dw dq = (2\pi)^n \text{Id} \quad (3.1)$$

holds, where $|\psi\rangle \langle \psi|$ is the Dirac notation for the orthogonal projection onto a normalized vector $\psi \in L^2(\mathbb{R}^n)$. Thanks to (3.1) and the fact that orthogonal projectors are nonnegative operators, we immediately obtain the following important estimate: for every nonnegative bounded function $\chi_\varepsilon : \mathbb{R}^{2n} \rightarrow \mathbb{R}$, it holds

$$\frac{1}{\varepsilon^n} \int_{\mathbb{R}^{2n}} \chi_\varepsilon(w, q) |\psi_{w,q}^\varepsilon\rangle \langle \psi_{w,q}^\varepsilon| dw dq \leq \|\chi_\varepsilon\|_\infty (2\pi)^n \text{Id}. \quad (3.2)$$

Set now

$$\tilde{\rho}_{0,\varepsilon} := \int_{\mathbb{R}^{2n}} \chi_\varepsilon(w, q) |\psi_{w,q}^\varepsilon\rangle \langle \psi_{w,q}^\varepsilon| dw dq, \quad \varepsilon \in (0, 1),$$

where $\{\chi_\varepsilon\}_{\varepsilon \in (0,1)}$ is a family of nonnegative bounded functions such that $\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w, q) dw dq = 1$, and let S be the singular set of U_s as defined in (4.23) below.

Proposition 3.2. *Let $\varsigma = \varsigma(\varepsilon) = \varepsilon^\alpha$ with $\alpha \in (0, 1)$, and assume that*

- $\sup_{\varepsilon \in (0,1)} \|\chi_\varepsilon\|_\infty < +\infty$.
- $w - \lim_{\varepsilon \rightarrow 0} \chi_\varepsilon \mathcal{L}^{2n} = \bar{\omega} \mathcal{L}^{2n} \in \mathcal{P}(\mathbb{R}^{2n})$
- $\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w, q) \left(|w|^4 + \frac{1}{\text{dist}(q, S)^2} \right) dw dq \leq C < +\infty$.

Then (2.10), (2.11), and (2.14) hold for the family of initial data $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$.

Proof. (2.11) follows from the first assumption and (3.2).

Since $\varsigma = \varepsilon^\alpha$ with $\alpha \in (0, 1)$ we have that for all $(w, q) \in \mathbb{R}^{2n}$

$$w - \lim_{\varepsilon \rightarrow 0} \tilde{W}_\varepsilon \psi_{w,q}^\varepsilon \mathcal{L}^{2n} = \delta_{(w,q)},$$

see [16, Exemple III.3], and so (2.14) follows from our second assumption.

To show that the third assumption implies (2.10), we notice that in this case (2.10) can be written as follows:

$$\sup_{\varepsilon \in (0,1)} \int_{\mathbb{R}^{2n}} \chi_\varepsilon(w, q) \langle H_\varepsilon \psi_{w,q}^\varepsilon, H_\varepsilon \psi_{w,q}^\varepsilon \rangle dw dq < +\infty. \quad (3.3)$$

Since $\alpha < 1$ and $\phi \in H^2(\mathbb{R}^n; \mathbb{C})$, by a simple computation we get

$$\begin{aligned} \langle H_\varepsilon \psi_{w,q}^\varepsilon, H_\varepsilon \psi_{w,q}^\varepsilon \rangle &\leq \frac{\varepsilon^4}{2} \langle \Delta_x \psi_{w,q}^\varepsilon, \Delta_x \psi_{w,q}^\varepsilon \rangle + 2 \langle U \psi_{w,q}^\varepsilon, U \psi_{w,q}^\varepsilon \rangle \\ &\leq C(1 + |w|^4) + C \int_{\mathbb{R}^n} U(x)^2 \frac{1}{\varsigma^n} \phi^2\left(\frac{x-q}{\varsigma}\right) dx. \end{aligned}$$

Since U_b is bounded, $|U_s(q)| \leq C/\text{dist}(q, S)$, and $\int_{\mathbb{R}^n} |\phi(x)|^2 dx = 1$, it is just a tedious computation (based on the fact that the convolution of $1/\text{dist}(q, S)^2$ with a sequence of mollifiers is still controlled by $C/\text{dist}(q, S)^2$) to prove (3.3). We leave the details to the interested reader. \square

3.3 Conditions on the Wigner function

Here we consider a general family of density matrices $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$ which satisfies the tightness conditions (2.12) and (2.13) (so that (2.14) is satisfied up to the extraction of a subsequence). In the next proposition we show some simple sufficient conditions on the Wigner functions $\{W_\varepsilon \rho_{0,\varepsilon}\}_{\varepsilon \in (0,1)}$ in order to ensure the validity of assumptions (2.10) and (2.11).

Proposition 3.3. *Assume that*

- $\max_{|\alpha|, |\beta| \leq 2[\frac{n}{2}]+2} \|\partial_x^\alpha \partial_p^\beta W_\varepsilon \rho_{0,\varepsilon}\|_\infty \leq C < +\infty,$
- $\int_{\mathbb{R}^{2n}} \left(\frac{|p|^4}{4} + U^2(x) + |p|^2 U(x) - \frac{n\varepsilon^2}{2} \Delta U(x) \right) W_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp \leq C < +\infty.$

Then (2.10) and (2.11) hold.

Proof. Let us recall first that the Weyl symbol of an operator $\tilde{\rho}$ of integral kernel $\rho(x, y)$ is, by definition, given by

$$\sigma_\varepsilon(\tilde{\rho})(x, p) := \int_{\mathbb{R}^n} \rho\left(x + \frac{y}{2}, x - \frac{y}{2}\right) e^{-iy \cdot p/\varepsilon} dy,$$

that is equal to $(2\pi\varepsilon)^n W_\varepsilon \rho$. Moreover, using (A.3) and (A.4), it holds

$$\mathrm{tr}(\tilde{\rho}) = \int_{\mathbb{R}^{2n}} W_\varepsilon \rho(x, p) dx dp \quad (3.4)$$

Hence, the first assumption gives (2.11) using Calderón-Vaillancourt Theorem [9].

Concerning (2.10), we now prove that

$$\sup_{\varepsilon \in (0,1)} \mathrm{tr}(H_\varepsilon^2 \tilde{\rho}_{0,\varepsilon}) < +\infty$$

(as observed in Section 2.3, this condition is slightly stronger than (2.10)). To this aim, we first note that

$$H_\varepsilon^2 = \frac{\varepsilon^4}{4} \Delta^2 + U^2 - \frac{\varepsilon^2}{2} \Delta U - \frac{\varepsilon^2}{2} U \Delta. \quad (3.5)$$

Moreover, let us observe that if $\tilde{\rho}_1$ and $\tilde{\rho}_2$ have kernels ρ_1 and ρ_2 respectively, then the kernel associated to the operator $\tilde{\rho}_1 \tilde{\rho}_2$ is given by $\int \rho_1(\cdot, z) \rho_2(z, \cdot) dz$. By this fact and (3.4), a simple computation shows that the identity

$$\mathrm{tr}(A \rho_\varepsilon) = \int_{\mathbb{R}^{2n}} \sigma_\varepsilon(A)(x, p) W_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp \quad (3.6)$$

holds for any ‘‘suitable’’ operator A (here $\sigma_\varepsilon(A)$ is the Weyl symbol of A).

Hence in this case

$$\mathrm{tr}(H_\varepsilon^2 \tilde{\rho}_\varepsilon) = \int_{\mathbb{R}^{2n}} \sigma_\varepsilon(H_\varepsilon^2)(x, p) W_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp.$$

We claim that the Weyl symbol of H_ε^2 is

$$\sigma_\varepsilon(H_\varepsilon^2)(x, p) = \frac{|p|^4}{4} + U^2(x) + |p|^2 U(x) - \frac{n\varepsilon^2}{2} \Delta U(x).$$

Indeed, let $f(x, p) := |p|^2 = \sigma_\varepsilon(-\varepsilon^2 \Delta)(x, p)$ and $g(x, p) := U(x) = \sigma_\varepsilon(U)(x, p)$. Then, using Moyal expansion,

$$\begin{aligned} \sigma_\varepsilon(H_\varepsilon^2)(x, p) &= \sigma_\varepsilon\left(\frac{\varepsilon^4}{4} \Delta^2 + U^2 - \frac{\varepsilon^2}{2} \Delta U - \frac{\varepsilon^2}{2} U \Delta\right)(x, p) \\ &= \frac{f(x, p)^2}{4} + g(x, p)^2 + \frac{1}{2} f \sharp g(x, p) + \frac{1}{2} g \sharp f(x, p), \end{aligned}$$

where by definition

$$h_1 \sharp h_2(x, p) := e^{i\frac{\varepsilon}{2}(\partial_x \partial_{p'} - \partial_p \partial_{x'})} h_1(x, p) h_2(x', p') \Big|_{x'=x, p'=p}.$$

In our case, in the expansion of the exponential

$$e^{i\frac{\varepsilon}{2}(\partial_x \partial_{p'} - \partial_p \partial_{x'})} = \sum_{j \in \mathbb{N}} \frac{1}{j!} \left(i\frac{\varepsilon}{2} (\partial_x \partial_{p'} - \partial_p \partial_{x'}) \right)^j$$

we can stop at the second order term, since $f(x, p) = |p|^2$. Therefore

$$f\sharp g(x, p) = |p|^2 U(x) - i\varepsilon p \cdot \nabla U(x) - \frac{n\varepsilon^2}{2} \Delta U(x),$$

and

$$g\sharp f(x, p) = |p|^2 U(x) + i\varepsilon p \cdot \nabla U(x) - \frac{n\varepsilon^2}{2} \Delta U(x).$$

This proves the claim and conclude the proof of the proposition. \square

4 Proof of Theorem 2.1

The proof of the theorem is split into several steps: first we show some basic estimates on the solutions, and we prove that the family $\tilde{W}_\varepsilon \rho_t^\varepsilon$ is tight in space and uniformly weakly continuous in time (this is the compactness part). Then we show that $\tilde{W}_\varepsilon \rho_t^\varepsilon$ solves the Liouville equation (away from the singular set of the Coulomb potential) with an error term which converges to zero as $\varepsilon \rightarrow 0$. Combining this fact with some uniform decay estimate for $\tilde{W}_\varepsilon \rho_t^\varepsilon$ away from the singularity, we finally prove that any limit point is bounded and solves the Liouville equation. By the uniqueness of solution to the Liouville equation in the function space $L_+^\infty([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$, we conclude the desired result.

Let us observe that some of our estimates can be found in [5] and [1]. However, the setting and the notation there are slightly different, and in some cases one would have to recheck the details of the proofs in [5, 1] to verify that everything works also in our case. Hence, for sake of completeness and in order to make this paper more accessible, we have decided to include all the details.

4.1 Basic estimates

4.1.1 Conserved quantities

The spectral decomposition of $\tilde{\rho}_t^\varepsilon$ is

$$\tilde{\rho}_t^\varepsilon = \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_{j,t}^{(\varepsilon)}, \cdot \rangle \phi_{j,t}^{(\varepsilon)},$$

where $\phi_{j,t}^{(\varepsilon)} = e^{-itH_\varepsilon/\varepsilon} \phi_j^{(\varepsilon)}$ solves (1.2). By standard results on the unitary propagator $e^{-itH_\varepsilon/\varepsilon}$ it follows that

$$\mathrm{tr}(H_\varepsilon \tilde{\rho}_{0,\varepsilon}) = \mathrm{tr}(H_\varepsilon \tilde{\rho}_t^\varepsilon) \quad (4.1)$$

and

$$\sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_{j,t}^{(\varepsilon)}\|^2 = \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_j^{(\varepsilon)}\|^2 \quad (4.2)$$

for all $t \in \mathbb{R}$ and $\varepsilon \in (0, 1)$. Therefore, using (4.1) and (2.10), we have

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \operatorname{tr}(H_\varepsilon \tilde{\rho}_t^\varepsilon) = \sup_{\varepsilon \in (0,1)} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)}, H_\varepsilon \phi_j^{(\varepsilon)} \rangle \leq \sqrt{c_1} < +\infty, \quad (4.3)$$

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_{j,t}^{(\varepsilon)}\|^2 = c_1 < +\infty. \quad (4.4)$$

4.1.2 A priori estimates

We now observe that the following a priori estimates hold:

$$\sup_{t \in \mathbb{R}} \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x, x) dx \leq \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_j^{(\varepsilon)}\|^2 + 2\|U_b\|_\infty \left(\operatorname{tr}(H_\varepsilon \tilde{\rho}_{0,\varepsilon}) + \|U_b\|_\infty \right) \quad (4.5)$$

and

$$\sup_{t \in \mathbb{R}} \frac{1}{2} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon \nabla \phi_{j,t}^{(\varepsilon)}(x)|^2 dx \leq \operatorname{tr}(H_\varepsilon \tilde{\rho}_{0,\varepsilon}) + \|U_b\|_\infty. \quad (4.6)$$

Here (4.6) is an easy consequence of (4.1), (4.2), and the positivity of U_s , while (4.5) follows from (4.1) and the fact that the real part of $\langle -\varepsilon^2 \Delta \phi_j^{(\varepsilon)}, U_s \phi_j^{(\varepsilon)} \rangle$ is nonnegative (see the proof of [5, Lemma 5.1]).

Hence, by (4.3) and (4.4) we obtain that

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x, x) dx \leq c_1 + 2\|U_b\|_\infty (\sqrt{c_1} + \|U_b\|_\infty) = C_1 < +\infty \quad (4.7)$$

and

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \frac{1}{2} \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon \nabla \phi_{j,t}^{(\varepsilon)}(x)|^2 dx \leq \sqrt{c_1} + \|U_b\|_\infty = C_2 < +\infty. \quad (4.8)$$

4.1.3 Propagation of (2.11) and consequences

Observe that, being $e^{itH_\varepsilon/\varepsilon}$ unitary, for all $t \in \mathbb{R}$ we have

$$\frac{1}{\varepsilon^n} \tilde{\rho}_t^\varepsilon \leq C \operatorname{Id}. \quad (4.9)$$

Hence, since

$$\tilde{W}_\varepsilon \rho_t^\varepsilon(y, p) = \frac{1}{(2\pi\varepsilon)^n} \langle \phi_{y,p}^\varepsilon, \tilde{\rho}_t^\varepsilon \phi_{y,p}^\varepsilon \rangle, \quad (4.10)$$

(see Appendix), using (4.9) we get

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \|\tilde{W}_\varepsilon \rho_t^\varepsilon\|_\infty \leq \frac{C}{(2\pi)^n} \|\phi_{y,p}^\varepsilon\|^2 = \frac{C}{(2\pi)^n} \quad (4.11)$$

(because $\|\phi_{y,p}^\varepsilon\| = 1$).

4.2 Tightness in space

Define $C_R^{(k)} = \{y = (y_1, \dots, y_k) \in \mathbb{R}^k : |y_j| \leq R, j = 1, \dots, k\}$. We want to prove that

$$\lim_{R \rightarrow +\infty} \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \int_{\mathbb{R}^{2n} \setminus C_R^{(2n)}} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp = 0. \quad (4.12)$$

Observe that for all $R > 0$

$$\begin{aligned} \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \int_{\mathbb{R}^{2n} \setminus C_R^{(2n)}} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp &\leq \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \frac{1}{2} \left[\int_{(\mathbb{R}^n \setminus C_R^{(n)}) \times \mathbb{R}^n} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \right. \\ &\quad \left. + \int_{\mathbb{R}^n \times (\mathbb{R}^n \setminus C_R^{(n)})} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \right], \end{aligned}$$

so we can check the tightness property separately for the first and the second marginals of $\tilde{W}_\varepsilon \rho_t^\varepsilon$. From (2.14) follows immediately that the family $\{\tilde{W}_\varepsilon \rho_{\varepsilon,0} \mathcal{L}^{2n}\}_{\varepsilon \in (0,1)}$ is tight (because, by Prokhorov's Theorem, a family of nonnegative finite measures on \mathbb{R}^{2n} is tight if and only if it is relatively compact in the duality with $C_b(\mathbb{R}^{2n})$). Therefore

$$\lim_{R \rightarrow +\infty} \int_{(\mathbb{R}^n \setminus C_R^{(n)}) \times \mathbb{R}^n} \tilde{W}_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp = 0. \quad (4.13)$$

Let $\chi \in C(\mathbb{R}^n)$, $0 \leq \chi \leq 1$ such that $\chi(x) = 0$ if $|x| < 1/2$ and $\chi(x) = 1$ if $|x| > 1$, and define $\chi_R(x) := \chi(x/R)$. Observe that $\|\nabla \chi_R\|_\infty \leq C'/R$ and $\|\Delta \chi_R\|_\infty \leq C'/R^2$. We define the following operator:

$$A_R^{(\varepsilon)} \psi(x) = \chi_R * G_\varepsilon^{(n)}(x) \psi(x), \quad \psi \in L^2(\mathbb{R}^n).$$

Observe that

$$\frac{d}{dt} \text{tr}(A_R^{(\varepsilon)} \tilde{\rho}_t^\varepsilon) = -\frac{i}{\varepsilon} \text{tr}([A_R^{(\varepsilon)}, H_\varepsilon] \tilde{\rho}_t^\varepsilon)$$

and that $[A_R^{(\varepsilon)}, H_\varepsilon] = \varepsilon^2 (\Delta(\chi_R * G_\varepsilon^{(n)})/2 + \nabla(\chi_R * G_\varepsilon^{(n)}) \cdot \nabla)$. So, using (4.8),

$$\begin{aligned} \frac{d}{dt} \text{tr}(A_R^{(\varepsilon)} \tilde{\rho}_t^\varepsilon) &= \frac{d}{dt} \int_{\mathbb{R}^{2n}} \chi_R(x) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \\ &\leq \frac{C'\varepsilon}{R^2} + \frac{C'\sqrt{C_2}}{R} \leq \frac{C'}{R^2} + \frac{C'\sqrt{C_2}}{R}, \end{aligned}$$

which gives

$$\begin{aligned} \int_{(\mathbb{R}^n \setminus C_{2R}^{(n)}) \times \mathbb{R}^n} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp &\leq \int_{\mathbb{R}^{2n}} \chi_R(x) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \\ &\leq \int_{\mathbb{R}^{2n}} \chi_R(x) \tilde{W}_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp + \left[\frac{C'}{R^2} + \frac{C'\sqrt{C_2}}{R} \right] T \\ &\leq \int_{(\mathbb{R}^n \setminus C_R^{(n)}) \times \mathbb{R}^n} \tilde{W}_\varepsilon \rho_{0,\varepsilon}(x, p) dx dp + \left[\frac{C'}{R^2} + \frac{C'\sqrt{C_2}}{R} \right] T. \end{aligned}$$

Therefore, using (4.13), we get

$$\lim_{R \rightarrow +\infty} \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \int_{(\mathbb{R}^n \setminus C_{2R}^{(n)}) \times \mathbb{R}^n} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp = 0, \quad (4.14)$$

as desired. For the second marginal we observe first that

$$\int_{\mathbb{R}^{2n}} |p|^2 \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp = \int_{\mathbb{R}^{2n}} |p|^2 W_\varepsilon \rho_t^\varepsilon(x, p) dx dp + \frac{n\varepsilon}{2} \quad (4.15)$$

and

$$\begin{aligned} \int_{\mathbb{R}^{2n}} |p|^2 W_\varepsilon \rho_t^\varepsilon(x, p) dx dp &= \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} \left| \frac{1}{(2\pi\varepsilon)^{n/2}} \hat{\phi}_{j,t}^{(\varepsilon)} \left(\frac{p}{\varepsilon} \right) \right|^2 |p|^2 dp \\ &= \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon \nabla \phi_{j,t}^{(\varepsilon)}(x)|^2 dx \end{aligned}$$

therefore, using (4.15) and (4.8), we have that

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \int_{\mathbb{R}^{2n}} |p|^2 \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \leq C_2 + \frac{n}{2} \quad (4.16)$$

and so

$$0 \leq \sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} \int_{\mathbb{R}^n \times (\mathbb{R}^n \setminus C_R^{(n)})} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \leq \frac{1}{R^2} \left(C_2 + \frac{n}{2} \right) \rightarrow 0 \quad \text{as } R \rightarrow +\infty.$$

4.3 Weak Lipschitz continuity in time

Here we prove that for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$ the map

$$t \in \mathbb{R} \mapsto f_{\varepsilon, \phi}(t) := \int_{\mathbb{R}^{2n}} \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp$$

is differentiable and

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in \mathbb{R}} \left| \frac{d}{dt} f_{\varepsilon, \phi}(t) \right| \leq C_\phi, \quad (4.17)$$

where C_ϕ is a constant depending only on ϕ . First observe that

$$f_{\varepsilon, \phi}(t) = \int_{\mathbb{R}^{2n}} W_\varepsilon \rho_t^\varepsilon(x, p) \phi_\varepsilon(x, p) dx dp,$$

where $\phi_\varepsilon := \phi * G_\varepsilon^{(2n)}$. Therefore, using (2.2), we have

$$\begin{aligned} \frac{d}{dt} f_{\varepsilon, \phi}(t) &= \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x, p) \phi_\varepsilon(x, p) dx dp \\ &\quad + \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon)(x, p) \phi_\varepsilon(x, p) dx dp \\ &\quad + \int_{\mathbb{R}^{2n}} (p \cdot \nabla_x \phi_\varepsilon(x, p)) W_\varepsilon \rho_t^\varepsilon(x, p) dx dp. \end{aligned} \quad (4.18)$$

For the first term it is easy to check that

$$\left| \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x, p) \phi_\varepsilon(x, p) dx dp \right| \leq \frac{\|\nabla U_b\|_\infty}{(2\pi)^n} \int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon|(x, y) dy. \quad (4.19)$$

In the case of the Coulomb potential we follow a specific argument borrowed from [5, proof of Theorem 1.1(ii)], based on the inequality

$$\left| \frac{1}{|z + w/2|} - \frac{1}{|z - w/2|} \right| \leq \frac{|w|}{|z + w/2||z - w/2|} \quad (4.20)$$

with $z = (x_i - x_j) \in \mathbb{R}^3$, $w = \varepsilon(y_i - y_j) \in \mathbb{R}^3$. By estimating the difference quotients of U_s as in (4.20), using (4.7) we obtain

$$\begin{aligned} \left| \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon)(x, p) \phi_\varepsilon(x, p) dx dp \right| &\leq C_* \int_{\mathbb{R}^n} |y| \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x', y)| dy \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x, x) dx \\ &\leq C_* C_1 \int_{\mathbb{R}^n} |y| \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x', y)| dy, \end{aligned} \quad (4.21)$$

with C_* depending only on the numbers Z_1, \dots, Z_M , and C_1 is the constant defined in (4.7).

For the last term it is easy to see that

$$\left| \int_{\mathbb{R}^{2n}} (p \cdot \nabla_x \phi_\varepsilon(x, p)) W_\varepsilon \rho_t^\varepsilon(x, p) dx dp \right| \leq \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon|(x', y) dy, \quad (4.22)$$

where

$$\tilde{\phi}_\varepsilon(x, p) = p \cdot \nabla_x \phi_\varepsilon(x, p).$$

Therefore, to conclude the proof of (4.17), we have only to bound

$$\int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x, y)| dy \quad \text{and} \quad \int_{\mathbb{R}^n} \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon|(x', y) dy$$

with a constant depending only on ϕ . The proof of these bounds is elementary, and is left to the reader.

4.4 Uniform decay away from the singularity

The singular set of U_s is given by

$$S = \bigcup_{1 \leq i < j \leq M} S_{ij}, \quad S_{ij} = \{x = (x_1, \dots, x_M, \bar{x}) \in (\mathbb{R}^3)^M \times \mathbb{R}^{n-3M} : x_i = x_j\}, \quad (4.23)$$

and we have

$$U_s(x) \geq \frac{c}{\text{dist}(x, S)}, \quad (4.24)$$

where $c > 0$ depends only on Z_1, \dots, Z_M . We want to prove that

$$\sup_{\delta > 0} \limsup_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{2n}} \left(|p|^4 + \frac{1}{\text{dist}(x, S)^2 + \delta} \right) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \leq C. \quad (4.25)$$

We start with the second term: observe that, for any $\delta > 0$,

$$\begin{aligned} \int_{\mathbb{R}^{2n}} \frac{1}{\text{dist}(x, S)^2 + \delta} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp &= \int_{\mathbb{R}^n} dx' \rho_t^\varepsilon(x', x') \int_{\mathbb{R}^n} dx \frac{G_\varepsilon^{(n)}(x)}{\text{dist}(x' - x, S)^2 + \delta} \\ &= \int_{\mathbb{R}^n} dx' \rho_t^\varepsilon(x', x') \int_{\mathbb{R}^n} dx \frac{G_1^{(n)}(x)}{\text{dist}(x' - \sqrt{\varepsilon}x, S)^2 + \delta}. \end{aligned} \quad (4.26)$$

and that

$$\int_{\mathbb{R}^n} \frac{G_1^{(n)}(x)}{\text{dist}(x' - \sqrt{\varepsilon}x, S)^2 + \delta} dx \rightarrow \frac{1}{\text{dist}(x', S)^2 + \delta} \quad \text{as } \varepsilon \rightarrow 0, \quad (4.27)$$

locally uniformly with respect to x' . Hence, since the family of functions $\{x' \mapsto \rho_t^\varepsilon(x', x')\}_{\varepsilon > 0}$ belongs to $L^1(\mathbb{R}^n)$ and is tight, it follows easily from (4.26), (4.27), (4.24), and (4.7), that for any $\delta > 0$

$$\begin{aligned} \limsup_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{2n}} \frac{1}{\text{dist}(x, S)^2 + \delta} \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp &\leq \limsup_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^n} \frac{\rho_t^\varepsilon(x', x')}{\text{dist}(x', S)^2 + \delta} dx' \\ &\leq \limsup_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^n} \frac{\rho_t^\varepsilon(x', x')}{\text{dist}(x', S)^2} dx' \\ &\leq \limsup_{\varepsilon \rightarrow 0} \frac{1}{c^2} \int_{\mathbb{R}^n} U_s^2(x') \rho_t^\varepsilon(x', x') dx' \leq \frac{C_1}{c^2} \end{aligned}$$

We now control the first term. We observe that

$$\begin{aligned} \int_{\mathbb{R}^{2n}} |p|^4 \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp &\leq \int_{\mathbb{R}^{2n}} |p|^4 W_\varepsilon \rho_t^\varepsilon(x, p) dx dp \\ &\quad + \frac{n\varepsilon}{2} \int_{\mathbb{R}^{2n}} |p|^2 W_\varepsilon \rho_t^\varepsilon(x, p) dx dp + \frac{n(n+2)\varepsilon^2}{4}. \end{aligned}$$

Of course, it suffices to control the first integral in the right hand side:

$$\begin{aligned} \int_{\mathbb{R}^{2n}} |p|^4 W_\varepsilon \rho_t^\varepsilon(x, p) dx dp &= \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} \left| \frac{1}{(2\pi\varepsilon)^{n/2}} \hat{\phi}_{j,t}^{(\varepsilon)} \left(\frac{p}{\varepsilon} \right) \right|^2 |p|^4 dp \\ &= \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon^2 \Delta \phi_{j,t}^{(\varepsilon)}(x)|^2 dx \\ &\leq 2 \sum_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} \left[|H_\varepsilon \phi_{j,t}^{(\varepsilon)}(x)|^2 + U^2(x) |\phi_{j,t}^{(\varepsilon)}(x)|^2 \right] dx, \end{aligned}$$

and the last term is uniformly bounded thanks to (4.4), (4.7), and the boundedness of U_b .

4.5 Limit continuity equation away from the singularities

We want to prove that

$$\lim_{\varepsilon \rightarrow 0} \int_0^T \left[\varphi'(t) \int_{\mathbb{R}^{2n}} \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp + \varphi(t) \int_{\mathbb{R}^{2n}} \mathbf{b}(x, p) \cdot \nabla \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \right] dt = 0 \quad (4.28)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n))$ and $\varphi \in C_c^\infty(0, T)$. Hence, recalling (2.6), we have to show that

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} dx dp \mathcal{E}_\varepsilon(U, \rho_t^\varepsilon) * G_\varepsilon^{(2n)}(x, p) \phi(x, p) + \int_{\mathbb{R}^{2n}} dx dp \nabla U(x) \cdot \nabla_p \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) = 0, \quad (4.29)$$

and

$$\lim_{\varepsilon \rightarrow 0} \int_0^T dt \varphi(t) \int_{\mathbb{R}^{2n}} dx dp \sqrt{\varepsilon} \nabla_x \cdot [W_\varepsilon \rho_t^\varepsilon * \tilde{G}_\varepsilon^{(2n)}] \phi(x, p) = 0, \quad (4.30)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n))$ and $\varphi \in C_c^\infty(0, T)$.

4.5.1 Verification of (4.29)

We can consider separately the contributions of U_b and U_s . We start with the contribution of U_s . We have to prove that

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} dx dp \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon) * G_\varepsilon^{(2n)}(x, p) \phi(x, p) + \int_{\mathbb{R}^{2n}} dx dp \nabla U_s(x) \cdot \nabla_p \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) = 0 \quad (4.31)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n))$.

We know that

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \left[\int_{\mathbb{R}^{2n}} \varphi(x, p) W_\varepsilon \rho_t^\varepsilon(x, p) dx dp - \int_{\mathbb{R}^{2n}} \varphi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \right] = 0 \quad (4.32)$$

for all $\varphi \in C_c^\infty(\mathbb{R}^{2n})$.

First of all, we see that we can apply (4.32) with $\varphi(x, p) = \nabla U_s(x) \cdot \nabla_p \phi(x, p)$ to replace the integrals

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon dx dp$$

with

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x, p) W_\varepsilon \rho_t^\varepsilon dx dp$$

in the verification of (4.31). Analogously, using (4.7) and (4.21) we see that we can replace

$$\int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon) * G_\varepsilon^{(2n)}(x, p) \phi(x, p) dx dp$$

with

$$\int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon)(x, p) \phi(x, p) dx dp.$$

Thus, we are led to show the convergence

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon) \phi \, dx \, dp + \int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x, p) W_\varepsilon \rho_t^\varepsilon(x, p) \, dx \, dp = 0 \quad (4.33)$$

for all $\phi \in C_c^\infty((\mathbb{R}^n \setminus S) \times \mathbb{R}^n)$. Since

$$\int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_s, \rho_t^\varepsilon) \phi \, dx \, dp = -\frac{i}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \frac{U_s(x + \frac{\varepsilon}{2}y) - U_s(x - \frac{\varepsilon}{2}y)}{\varepsilon} \rho_t^\varepsilon\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right) \mathcal{F}_p \phi(x, y) \, dx \, dy$$

we can split the region of integration in two parts, where $\sqrt{\varepsilon}|y| > 1$ and where $\sqrt{\varepsilon}|y| \leq 1$. The contribution of the first region can be estimated as in (4.21), with

$$C_* \int_{\{\sqrt{\varepsilon}|y| > 1\}} |y| \sup_{x'} |\mathcal{F}_p \phi(x', y)| \, dy \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x, x) \, dx,$$

which is infinitesimal, using (4.7) again, as $\varepsilon \rightarrow 0$. Since

$$\frac{U_s(x + \frac{\varepsilon}{2}y) - U_s(x - \frac{\varepsilon}{2}y)}{\varepsilon} \rightarrow \nabla U_s(x) \cdot y$$

uniformly as $\sqrt{\varepsilon}|y| \leq 1$ and x belongs to a compact subset of $\mathbb{R}^n \setminus S$, the contribution of the second part is the same of

$$-\frac{i}{(2\pi)^n} \int_{\mathbb{R}^{2n}} (\nabla U_s(x) \cdot y) \rho_t^\varepsilon\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right) \mathcal{F}_p \phi(x, y) \, dx \, dy$$

which coincides with

$$-\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x, p) W_\varepsilon \rho_t^\varepsilon(x, p) \, dx \, dp.$$

Now we consider the contribution of U_b . We have to prove that

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x, p) \phi_\varepsilon(x, p) \, dx \, dp + \int_{\mathbb{R}^{2n}} \nabla U_b(x) \cdot \nabla_p \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon \, dx \, dp = 0 \quad (4.34)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$, where $\phi_\varepsilon = \phi * G_\varepsilon^{(2n)}$. The proof of (4.34) is divided in two parts: first we prove that

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x, p) \phi(x, p) \, dx \, dp + \int_{\mathbb{R}^{2n}} \nabla U_b(x) \cdot \nabla_p \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon \, dx \, dp = 0 \quad (4.35)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$, and then, using the following estimate

$$\left| \int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x, p) \phi(x, p) \, dx \, dp \right| \leq \frac{\|\nabla U_b\|_\infty}{(2\pi)^n} \int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} |\mathcal{F}_p \phi|(x, y) \, dy. \quad (4.36)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$, we can replace ϕ by ϕ_ε in the first summand of (4.35), obtaining (4.34). The proof of (4.35) is achieved by a density argument. The first remark is that linear combinations

of tensor functions $\phi(x, p) = \phi_1(x)\phi_2(p)$, with $\phi_i \in C_c^\infty(\mathbb{R}^n)$, are dense for the norm considered in (4.36). In this way, we are led to prove convergence in the case when $\phi(x, p) = \phi_1(x)\phi_2(p)$. The second remark is that convergence surely holds if U_b is of class C^2 (by the arguments in [16], [5]). Hence, combining the two remarks and using the linearity of the error term with respect to the potential, we can prove convergence by a density argument, by approximating U_b uniformly and in $W^{1,2}$ topology on the support of ϕ_1 by potentials in $C^2(\mathbb{R}^n)$. Therefore, to obtain (4.35) we only need to prove that the left hand side is continuous in $L^\infty \cap W^{1,2}$ topology.

To show this, we observe that

$$\int_{\mathbb{R}^{2n}} \mathcal{E}_\varepsilon(U_b, \rho_t^\varepsilon) \phi_1(x) \phi_2(p) dx dp = I_{\varepsilon,t} + II_{\varepsilon,t} + III_{\varepsilon,t},$$

where

$$\begin{aligned} I_{\varepsilon,t} &:= \int_{\mathbb{R}^{2n}} \frac{A(x + \frac{\varepsilon}{2}y) - A(x - \frac{\varepsilon}{2}y)}{\varepsilon} \hat{\phi}_2(y) \rho_t^\varepsilon(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) dx dy, \\ II_{\varepsilon,t} &:= \int_{\mathbb{R}^{2n}} U_b(x + \frac{\varepsilon}{2}y) \frac{\phi_1(x) - \phi_1(x + \frac{\varepsilon}{2}y)}{\varepsilon} \hat{\phi}_2(y) \rho_t^\varepsilon(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) dx dy, \\ III_{\varepsilon,t} &:= - \int_{\mathbb{R}^{2n}} U_b(x - \frac{\varepsilon}{2}y) \frac{\phi_1(x) - \phi_1(x - \frac{\varepsilon}{2}y)}{\varepsilon} \hat{\phi}_2(y) \rho_t^\varepsilon(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) dx dy. \end{aligned}$$

and $A = U_b \phi_1$. Observe that

$$\sup_{\varepsilon \in (0,1)} \sup_{t \in [0,T]} |II_{\varepsilon,t}| + |III_{\varepsilon,t}| \leq \|U_b\|_\infty \|\nabla \phi_1\|_\infty \int_{\mathbb{R}^n} |y| |\hat{\phi}_2(y)| dy.$$

For estimating of $I_{\varepsilon,t}$ we observe first that

$$\begin{aligned} \int_{\mathbb{R}^{2n}} \left| \rho_t^\varepsilon \left(x + \varepsilon \frac{y}{2}, x - \varepsilon \frac{y}{2} \right) \right|^2 dx dy &= \frac{1}{\varepsilon^n} \int_{\mathbb{R}^{2n}} |\rho_t^\varepsilon(z, z')|^2 dz dz' \\ &= \frac{1}{\varepsilon^n} \sum_{j \in \mathbb{N}} \left(\mu_j^{(\varepsilon)} \right)^2 \leq \frac{1}{\varepsilon^n} \sup_{j \in \mathbb{N}} \mu_j^{(\varepsilon)} \sum_{k \in \mathbb{N}} \mu_k^{(\varepsilon)} \leq C. \end{aligned}$$

Thus, applying the Cauchy-Schwartz inequality to $I_{\varepsilon,t}$ (both in x and y) and using the fundamental theorem of calculus to estimate the incremental quotients, we easily obtain

$$|I_{\varepsilon,t}| \leq \frac{C}{(2\pi)^n} \|\nabla A\|_2 \left(\int_{\mathbb{R}^n} |y|^2 |\hat{\phi}_2(y)|^2 dy \right)^{1/2},$$

which proves the result.

4.5.2 Verification of (4.30)

This is easy, taking into account the fact that

$$\int_{\mathbb{R}^{2n}} W_\varepsilon \rho_t^\varepsilon * \bar{G}_\varepsilon^{(2n)}(x, p) \cdot \nabla_x \phi(x, p) dx dp = \int_{\mathbb{R}^{2n}} W_\varepsilon \rho_t^\varepsilon \nabla_x \cdot [\phi * \bar{G}_\varepsilon^{(2n)}] dx dp$$

are uniformly bounded (where $\bar{G}_\varepsilon^{(2n)}$ is defined in (2.7)).

4.6 Proof of Theorem 2.1

Define $\mathcal{W}^{(\varepsilon)} : [0, T] \rightarrow \mathcal{P}(\mathbb{R}^{2n})$ as $\mathcal{W}_t^{(\varepsilon)} := \tilde{W}_\varepsilon \rho_t^\varepsilon \mathcal{L}^{2n}$ for all $\varepsilon \in (0, 1)$ and $t \in [0, T]$. Using (4.12), (4.17) and Ascoli-Arzelà Theorem, one can prove easily that there exists a subsequence $\{\mathcal{W}^{(\varepsilon_k)}\}_{k \in \mathbb{N}}$ and $W : [0, T] \rightarrow \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\lim_{k \rightarrow \infty} \sup_{t \in [0, T]} d_{\mathcal{P}}(\mathcal{W}_t^{(\varepsilon_k)}, W_t) = 0. \quad (4.37)$$

We now prove the following assertions:

- (i) $W : [0, T] \rightarrow \mathcal{P}(\mathbb{R}^{2n})$ is weakly continuous and, for all $t \in [0, T]$, $W_t = \tilde{\mathcal{W}}_t \mathcal{L}^{2n}$ for some function $\tilde{\mathcal{W}}_t \in L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$. Moreover $\tilde{\mathcal{W}}_t \geq 0$ and $\sup_{t \in [0, T]} \|\tilde{\mathcal{W}}_t\|_{L^1(\mathbb{R}^{2n})} + \|\tilde{\mathcal{W}}_t\|_{L^\infty(\mathbb{R}^{2n})} \leq C$. In particular, $\tilde{\mathcal{W}} \in L^1_+(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$.
- (ii) $\mathbf{b} \in L^1_{\text{loc}}((0, T) \times \mathbb{R}^{2n}; dt dW_t)$, so the continuity equation (2.8) with $\omega_t = \tilde{\mathcal{W}}_t$ makes sense;
- (iii) W solves (2.8) in the sense of distributions on $[0, T] \times \mathbb{R}^{2n}$;
- (iv) For any $\phi \in C_c^\infty(\mathbb{R}^{2n})$, $t \mapsto \int_{\mathbb{R}^{2n}} \phi dW_t$ belongs to $C^1([0, T])$.

Proof of (i): Observe that (4.37) implies that $W : [0, T] \rightarrow \mathcal{P}(\mathbb{R}^{2n})$ is weakly continuous because it is uniform limit of the weakly continuous maps $\mathcal{W}^{(\varepsilon_k)}$. The second part of the proposition follows immediately from (4.11). Indeed, for all $\phi \in L^1(\mathbb{R}^{2n})$,

$$\sup_{\varepsilon \in (0, 1)} \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \phi(x, p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x, p) dx dp \leq \frac{C}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \phi(x, p) dx dp \quad (4.38)$$

and so

$$\sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \phi(x, p) dW_t(x, p) \leq \frac{C}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \phi(x, p) dx dp. \quad (4.39)$$

Proof of (ii): We observe that, thanks to (4.25) and the monotone convergence theorem,

$$\sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \frac{1}{\text{dist}(x, S)^2} dW_t(x, p) = \sup_{t \in [0, T]} \sup_{\delta > 0} \int_{\mathbb{R}^{2n}} \frac{1}{\text{dist}(x, S)^2 + \delta} dW_t(x, p) < +\infty. \quad (4.40)$$

Hence, the estimate $\mathbf{b} \in L^1_{\text{loc}}((0, T) \times \mathbb{R}^{2n}; dW_t dt)$ follows immediately from (4.40) and (4.16).

Proof of (iii): First we prove that $\tilde{\mathcal{W}}$ solves (2.8) in $\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n)$, where S is the singular set of U_s defined in (4.23). Unfortunately this does not follow immediately by (4.28) because we have no information about the singular set Σ of ∇U_b , so we cannot control the limit $k \rightarrow \infty$ of

$$\int_0^T dt \varphi(t) \int_{\mathbb{R}^{2n}} dx dp \nabla U_b(x) \cdot \nabla_p \phi(x, p) \tilde{W}_{\varepsilon_k} \rho_t^{\varepsilon_k}(x, p)$$

in (2.8) with (4.37). But we can proceed by a density argument because, using the regularity conditions (4.38) and (4.39), we can approximate ∇U_b in L^1 on $\text{supp} \phi$ by bounded continuous functions.

In order to prove that $\tilde{\mathcal{W}}$ solves (2.8) in $[0, T] \times \mathbb{R}^{2n}$, we observe that (4.40) implies that $W_t(S \times \mathbb{R}^n) = 0$ for every $t \in (0, T)$. Hence, the proof of the global validity of the continuity equation uses the classical argument of removing the singularity by multiplying any test function $\phi \in C_c^\infty(\mathbb{R}^{2n})$ by χ_k , where $\chi_k(x) = \chi(k \text{dist}(x, S))$ and χ is a smooth cut-off function equal to 0 on $[0, 1]$ and equal to 1 on $[2, +\infty)$, with $0 \leq \chi' \leq 2$. Indeed, if we use $\phi \chi_k$ as a test function, since χ_k depends on x only, we can use the particular structure of \mathbf{b} , namely $\mathbf{b}(x, p) = (p, -\nabla U(x))$, to write the term depending on the derivatives of χ_k as

$$k \int_{\mathbb{R}^{2n}} \phi \chi'(k \text{dist}(x, S)) p \cdot \nabla \text{dist}(x, S) dW_t(x, p) dt.$$

If K is the support of ϕ , the integral above can be bounded by

$$2 \sup_K |p\phi| \int_{\{x \in K : k \text{dist}(x, S) \leq 2\}} k dW_t(x, p) dt \leq \frac{8 \max_K |p\phi|}{k} \int_K \frac{1}{\text{dist}^2(x, S)} dW_t(x, p),$$

and by (4.40) the right hand side is infinitesimal (uniformly in t) as $k \rightarrow \infty$.

Proof of (iv): Since the distributional derivative of $t \mapsto \int_{\mathbb{R}^{2n}} \phi W_t dx dp$ is given by $\int_{\mathbb{R}^{2n}} \mathbf{b} \cdot \nabla \phi dW_t$, we have to show that the map

$$t \mapsto \int_{\mathbb{R}^{2n}} \mathbf{b} \cdot \nabla \phi dW_t$$

is continuous. Observing that the map $t \mapsto W_t$ is weakly continuous and $W_t = \tilde{\mathcal{W}}_t \mathcal{L}^{2n}$ with $\tilde{\mathcal{W}} \in L_+^\infty([0, T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$, the only delicate term is

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x, p) dW_t.$$

Define the nonnegative Hamiltonian function $\mathcal{H} = |p|^2/2 + U + \|U_b\|_\infty$. Taking the limit in (4.25) (first as $\varepsilon \rightarrow 0$ and then as $\delta \rightarrow 0$) we easily deduce that

$$\sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \mathcal{H}^2 dW_t \leq C \sup_{t \in [0, T]} \int_{\mathbb{R}^{2n}} \left(1 + |p|^4 + U_s^2(x)\right) dW_t < +\infty.$$

Since the Hamiltonian is preserved by the Liouville dynamics (under our assumptions on the potential, this fact is contained in the proof of [1, Theorem 6.1]), the above bound gives

$$\sup_{t \in [0, T]} \int_{\{\mathcal{H} \geq N\}} \mathcal{H}^2 dW_t = \int_{\{\mathcal{H} \geq N\}} \mathcal{H}^2 dW_0 \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

As $U_s \leq \mathcal{H}$, this implies

$$\sup_{t \in [0, T]} \int_{\{U_s \geq N\}} U_s^2 dW_t \leq \int_{\{\mathcal{H} \geq N\}} \mathcal{H}^2 dW_0 \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Hence, if we define the sets $A_N := \{U_s \leq N\}$, the functions

$$t \mapsto f_N(t) := \int_{A_N} \nabla U_s(x) \cdot \nabla_p \phi dW_t$$

are continuous and converge uniformly to $\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi dW_t$ as $N \rightarrow \infty$. This proves (iv).

To conclude the proof of the theorem, recalling that \mathscr{W} denote the unique distributional solution of (2.8) in $L^{\infty}_+([0, T]; L^1(\mathbb{R}^{2n}) \cap L^{\infty}(\mathbb{R}^{2n}))$ starting from $\tilde{\omega} \mathcal{L}^{2n}$ (see [1, Theorem 6.1]), we have proved $\tilde{\mathscr{W}} = \mathscr{W}$, and so

$$\lim_{k \rightarrow \infty} \sup_{t \in [0, T]} d_{\mathcal{D}}(\tilde{W}_{\varepsilon_k} \rho_t^{\varepsilon_k} \mathcal{L}^{2n}, \mathscr{W}_t \mathcal{L}^{2n}) = 0. \quad (4.41)$$

Since the limit $\mathscr{W}_t \mathcal{L}^{2n}$ is independent of the chosen subsequence, this implies the convergence of the whole family, namely

$$\lim_{\varepsilon \rightarrow 0} \sup_{t \in [0, T]} d_{\mathcal{D}}(\tilde{W}_{\varepsilon} \rho_t^{\varepsilon} \mathcal{L}^{2n}, \mathscr{W}_t \mathcal{L}^{2n}) = 0, \quad (4.42)$$

as desired.

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A Notation and some notions about density operators

A density operator on $L^2(\mathbb{R}^n)$ is a positive, self-adjoint, trace-class operator, namely $\tilde{\rho} = \tilde{\rho}^*$, $\tilde{\rho} \geq 0$, and $\text{tr}(\tilde{\rho}) = 1$, where the trace is defined as follows:

$$\text{tr}(\tilde{\rho}) := \sum_{j \in \mathbb{N}} \langle \varphi_j, \tilde{\rho} \varphi_j \rangle \quad (A.1)$$

with $\{\varphi_j\}_{j \in \mathbb{N}}$ any orthonormal basis of $L^2(\mathbb{R}^n)$. It can be shown that each density operator $\tilde{\rho}$ is a compact operator, so it can be decomposed as follows

$$\tilde{\rho} = \sum_{j \in \mathbb{N}} \lambda_j \langle \psi_j, \cdot \rangle \psi_j \quad (A.2)$$

where $1 \geq \lambda_1 \geq \lambda_2 \geq \dots \geq 0$, and $\{\psi_j\}_{j \in \mathbb{N}}$ is a orthonormal basis of eigenvectors of $\tilde{\rho}$. Therefore $\tilde{\rho}$ is an integral operator and its kernel is

$$\rho(x, y) = \sum_{j \in \mathbb{N}} \lambda_j \psi_j(x) \overline{\psi_j(y)},$$

so that

$$\tilde{\rho}\psi(x) = \int_{\mathbb{R}^n} \rho(x, y)\psi(y) dy.$$

Observe that the trace condition on $\tilde{\rho}$ can be expressed as follows in terms of its kernel

$$\mathrm{tr}(\tilde{\rho}) = \int_{\mathbb{R}^n} \rho(x, x) dx = 1. \quad (\text{A.3})$$

The Wigner transform of ρ is defined as

$$W_\varepsilon\rho(x, p) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \rho\left(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y\right) e^{-ipy} dy,$$

and the Husimi transform of ρ as

$$\tilde{W}_\varepsilon\rho := W_\varepsilon\rho * G_\varepsilon^{(2n)}, \quad G_\varepsilon^{(2n)}(x, p) := G_\varepsilon^{(n)}(x)G_\varepsilon^{(n)}(p) = \frac{e^{-\frac{(|x|^2+|p|^2)}{\varepsilon}}}{(\pi\varepsilon)^n}.$$

It is easy to check that the marginals of $W_\varepsilon\rho$ are

$$\int_{\mathbb{R}^n} W_\varepsilon\rho(x, p) dp = \rho(x, x) \quad \text{and} \quad \int_{\mathbb{R}^n} W_\varepsilon\rho(x, p) dx = \frac{1}{(2\pi\varepsilon)^n} \mathcal{F}\rho\left(\frac{p}{\varepsilon}, \frac{p}{\varepsilon}\right) \quad (\text{A.4})$$

where

$$\mathcal{F}\rho(q, q) = \int_{\mathbb{R}^{2n}} \rho(u, u) e^{-iq \cdot (u-v)} dudv. \quad (\text{A.5})$$

Similarly the marginals of $\tilde{W}_\varepsilon\rho$ are

$$\int_{\mathbb{R}^n} \tilde{W}_\varepsilon\rho(x, p) dp = \int_{\mathbb{R}^n} \rho(x - x', x - x') G_\varepsilon^{(n)}(x') dx' \quad (\text{A.6})$$

and

$$\int_{\mathbb{R}^n} \tilde{W}_\varepsilon\rho(x, p) dx = \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \mathcal{F}\rho\left(\frac{p-p'}{\varepsilon}, \frac{p-p'}{\varepsilon}\right) G_\varepsilon^{(n)}(p') dp'. \quad (\text{A.7})$$

Moreover, the Husimi transform is nonnegative: indeed (see for instance [16]),

$$\tilde{W}_\varepsilon\rho(x, p) = \frac{1}{(2\pi\varepsilon)^n} |\langle \psi, \phi_{x,p}^\varepsilon \rangle|^2, \quad (\text{A.8})$$

where $\langle \cdot, \cdot \rangle$ is the scalar product on $L^2(\mathbb{R}^n)$ and

$$\phi_{x,p}^\varepsilon(y) := \frac{1}{(\pi\varepsilon)^{n/4}} e^{-|x-y|^2/(2\varepsilon)} e^{ipy/\varepsilon} \in L^2(\mathbb{R}^n), \quad \|\phi_{x,p}^\varepsilon\| = 1.$$

Hence $\tilde{W}_\varepsilon\psi \geq 0$, and using the spectral decomposition (A.2) one obtains the non-negativity of $\tilde{W}_\varepsilon\rho$ for any trace-class operator ρ . Moreover, combining (A.3) and (A.6), it follows that $\tilde{W}_\varepsilon\rho$ is a probability measure.

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