Semiclassical Limit of Quantum Dynamics with Rough Potentials and Well-Posedness of Transport Equations with Measure Initial Data

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Abstract

In this paper we study the semiclassical limit of the Schrödinger equation. Under mild regularity assumptions on the potential U, which include Born-Oppenheimer potential energy surfaces in molecular dynamics, we establish asymptotic validity of classical dynamics globally in space and time for "almost all" initial data, with respect to an appropriate reference measure on the space of initial data. In order to achieve this goal we prove existence, uniqueness, and stability results for the flow in the space of measures induced by the continuity equation.
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1 Introduction

In this paper we study the semiclassical limit of the Schrödinger equation. Under mild regularity assumptions on the potential U, which include Born-Oppenheimer potential energy surfaces in molecular dynamics, we establish asymptotic validity of classical dynamics globally in space and time for "almost all" initial data, with respect to an appropriate reference measure on the space of initial data. In order to achieve this goal, we study the flow in the space of measures induced by the continuity equation: we prove existence, uniqueness, and stability properties of the flow in this infinite-dimensional space, in the same spirit as the theory developed in the case when the state space is euclidean, starting from the seminal paper [13] (see also [1] and the lecture notes [2, 3]).

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As we said, we are concerned with the derivation of classical mechanics from quantum mechanics, corresponding to the study of the asymptotic behavior of solutions $\psi^\varepsilon(t,x) = \psi_t^\varepsilon(x)$ to the Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t \psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi_t^\varepsilon + U\psi_t^\varepsilon = H_\varepsilon\psi_t^\varepsilon, \\ \psi_0^\varepsilon = \psi_{0,\varepsilon}, \end{cases} \tag{1.1}$$

as $\varepsilon \to 0$. This problem has a long history (see, e.g., [25]) and has been considered from a transport equation point of view in [20, 24] and more recently in [6] in the context of molecular dynamics. In that context the standing assumptions on the initial conditions $\psi_{0,\varepsilon} \in H^2(\mathbb{R}^n;\mathbb{C})$ are:

$$\int_{\mathbb{R}^n} |\psi_{0,\varepsilon}|^2\,dx = 1, \tag{1.2}$$

$$\sup_{\varepsilon>0} \int_{\mathbb{R}^n} |H_\varepsilon\psi_{0,\varepsilon}|^2\,dx < \infty. \tag{1.3}$$

The potential U in (1.1) can be represented by the form $U_b + U_s$, where U_s is assumed to satisfy the standard Kato condition

$$U_s(x) = \sum_{1\le\alpha<\beta\le M} V_{\alpha\beta}(x_\alpha - x_\beta), \qquad V_{\alpha\beta} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3), \tag{1.4}$$

and

$$U_b \in L^\infty(\mathbb{R}^n), \tag{1.5}$$

$$\nabla U_b \in L^\infty(\mathbb{R}^n;\mathbb{R}^n). \tag{1.6}$$

Here $n = 3M$ and $x = (x_1,\dots,x_M) \in (\mathbb{R}^3)^M$ represent the positions of atomic nuclei. Under assumptions (1.4) and (1.5) the operator H_ε is self-adjoint on $L^2(\mathbb{R}^n;\mathbb{C})$ with domain $H^2(\mathbb{R}^n;\mathbb{C})$ and generates a unitary group in $L^2(\mathbb{R}^n;\mathbb{C})$; hence $\int_{\mathbb{R}^n} |\psi_t^\varepsilon|^2\,dx = 1$ for all $t \in \mathbb{R}$, and $t \mapsto \psi_t^\varepsilon$ is continuous with values in $H^2(\mathbb{R}^n;\mathbb{C})$ and continuously differentiable with values in $L^2(\mathbb{R}^n;\mathbb{C})$. Prototypically, U is the Born-Oppenheimer ground state potential energy surface of the molecule, that is to say,

$$U_s = \sum_{1\le\alpha<\beta\le M} \frac{Z_\alpha Z_\beta}{|x_\alpha - x_\beta|}, \quad Z_1,\dots,Z_M > 0, \tag{1.7}$$

$$U_b(x) = \inf\operatorname{spec} H_{e\ell}(x), \tag{1.8}$$

where the Z_α are the charges of the nuclei,

$$H_{e\ell}(x) = \sum_{i=1}^N \left(-\frac{1}{2}\Delta_{r_i} - \sum_{\alpha=1}^M Z_\alpha |r_i - x_\alpha|^{-1}\right) + \sum_{1\le i<j\le N} |r_i - r_j|^{-1} \tag{1.9}$$

is the electronic Hamiltonian acting on the antisymmetric subspace of $L^2((\mathbb{R}^3 \times \mathbb{Z}_2)^N; \mathbb{C})$, and the $r_i \in \mathbb{R}^3$ are electronic position coordinates. Here N is the number of electrons in the system, which typically equals $Z_1 + \cdots + Z_M$.

In the study of this semiclassical limit, difficulties arise on the one hand from the fact that ∇U is unbounded (because of Coulomb singularities) and on the other hand from the fact that ∇U might be discontinuous even out of Coulomb singularities (because of possible eigenvalue crossings of the electronic Hamiltonian $H_{e\ell}$). These singularities mean that the classical flow that formally emerges in the limit, i.e., the flow generated by the ODE

$$\frac{d}{dt}\begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} p \\ -\nabla U(x) \end{pmatrix}, \tag{1.10}$$

is not even well-posed—standard ODE theory would require ∇U to be Lipschitz.

The fact that we are able to overcome this lack of smoothness relies on three recent developments and observations: First, the recent "almost everywhere" existence and uniqueness results [1, 3] for ODEs in $\mathbb{R}^d$ with vector field in BV, which we extend to the case when the state space is $\mathscr{P}(\mathbb{R}^d)$, the space of Borel probability measures in $\mathbb{R}^d$ (see also [5]). Second, we exploit the observation in [19] that for Born-Oppenheimer potential energy surfaces U given by (1.7)–(1.9), ∇U (and hence the vector field in (1.10)) lies exactly in BV away from Coulomb singularities (see Proposition 7.1). Third, we adapt the method introduced in [6] for dealing with Coulomb singularities when the remaining part of the potential is smooth. Finally, we prove new nontrivial a priori estimates for solutions to (1.1) (see Section 7) in order to be able to apply our theory of flows in $\mathscr{P}(\mathbb{R}^d)$.

The natural setting for "almost everywhere" uniqueness of the classical flow generated by (1.10) is that of the corresponding Liouville equation. If we denote by $\boldsymbol{b} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ the autonomous divergence-free vector field $\boldsymbol{b}(x, p) := (p, -\nabla U(x))$, the Liouville equation is

$$\partial_t \mu_t + p \cdot \nabla_x \mu_t - \nabla U(x) \cdot \nabla_p \mu_t = 0. \tag{1.11}$$

If we denote by $W_\varepsilon : L^2(\mathbb{R}^n; \mathbb{C}) \to L^\infty(\mathbb{R}^n_x \times \mathbb{R}^n_p)$ the Wigner transform, namely

$$W_\varepsilon \psi(x, p) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \psi\left(x + \frac{\varepsilon}{2} y\right) \overline{\psi\left(x - \frac{\varepsilon}{2} y\right)} e^{-ipy}\, dy, \tag{1.12}$$

a calculation going back to Wigner himself (see, for instance, [6] or [24] for a detailed derivation) shows that if ψ_t^ε solves (1.1), then $W_\varepsilon \psi_t^\varepsilon$ solves in the sense of distributions the equation

$$\partial_t W_\varepsilon \psi_t^\varepsilon + p \cdot \nabla_x W_\varepsilon \psi_t^\varepsilon = \mathscr{E}_\varepsilon(U, \psi_t^\varepsilon), \tag{1.13}$$

where $\mathscr{E}_\varepsilon(U,\psi)(x,p)$ is given by

$$\text{(1.14)} \quad \mathscr{E}_\varepsilon(U,\psi)(x,p) := -\frac{i}{(2\pi)^n}\int_{\mathbb{R}^n}\left[\frac{U(x+\frac{\varepsilon}{2}y)-U(x-\frac{\varepsilon}{2}y)}{\varepsilon}\right]\psi\left(x+\frac{\varepsilon}{2}y\right)\overline{\psi\left(x-\frac{\varepsilon}{2}y\right)}e^{-ipy}\,dy.$$

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

$$\text{(1.15)} \quad \mathscr{E}'_\varepsilon(U,\psi)(x,p) := -\frac{i}{(2\pi)^n}\int_{\mathbb{R}^n}\left[\frac{U(x+\frac{\varepsilon}{2}y)-U(x-\frac{\varepsilon}{2}y)}{\varepsilon} - \langle\nabla U(x),y\rangle\right] \times\psi\left(x+\frac{\varepsilon}{2}y\right)\overline{\psi(x-\frac{\varepsilon}{2}y)}e^{-ipy}\,dy.$$

Hence, $W_\varepsilon\psi_t^\varepsilon$ solves (1.11) with an error term,

$$\partial_t W_\varepsilon\psi_t^\varepsilon + \nabla_{x,p}\cdot(\boldsymbol{b}W_\varepsilon\psi_t^\varepsilon) = \mathscr{E}'_\varepsilon(U,\psi_t^\varepsilon). \tag{1.16}$$

Heuristically, since the term in square brackets in (1.15) tends to 0 when U is differentiable, this suggests that the limit of $W_\varepsilon\psi_t^\varepsilon$ should satisfy (1.11), and a first rigorous proof of this fact was given in [20, 24] (see also [21]): basically, ignoring other global conditions on U and assuming initial conditions of appropriate wavelength (see (1.3) and (1.17)), these results state that:

(1) C^1 regularity of U ensures that limit points of $W_\varepsilon\psi_t^\varepsilon$ as $\varepsilon\downarrow 0$ (i) exist and (ii) satisfy (1.11);
(2) C^2 regularity of U ensures uniqueness of the limit, i.e., full convergence as $\varepsilon\to 0$.

In (1), convergence of the Wigner transforms is understood in a natural dual space $\mathcal{A}'$ (see (7.5) for the definition of $\mathcal{A}$). In [6] we were able to achieve (1)(i) even when Coulomb singularities and crossings are present, namely, assuming only that U_b satisfies (1.5) and (1.6); and to achieve (1)(ii) when Coulomb singularities but no crossings are present, namely, assuming that $U_b\in C^1$. If one wishes to improve (1)(ii) and (2), trying to prove a full convergence result as $\varepsilon\downarrow 0$ under weaker regularity assumptions on $\boldsymbol{b}$ (say $\nabla U\in W^{1,p}$ or $\nabla U\in \mathrm{BV}$ out of Coulomb singularities), one faces the difficulty that the continuity equation (1.11) is well-posed only in good functional spaces like $L^\infty_+([0,T];L^1\cap L^\infty(\mathbb{R}^d))$ (see [1, 12, 13]). On the other hand, in the study of semiclassical limits it is natural to consider families of wave functions $\psi_{0,\varepsilon}$ in (1.1) whose Wigner transforms do concentrate as $\varepsilon\downarrow 0$, for instance, the semiclassical wave packets

$$\psi_{0,\varepsilon}(x) = \varepsilon^{-n\alpha/2}\phi_0\left(\frac{x-x_0}{\varepsilon^\alpha}\right)e^{i(x\cdot p_0)/\varepsilon}, \quad \phi_0\in C_c^2(\mathbb{R}^n),\ 0<\alpha<1, \tag{1.17}$$

which satisfy $\lim_\varepsilon W_\varepsilon\psi_{0,\varepsilon} = \|\phi_0\|_2^2\delta_{(x_0,p_0)}$. Here the limiting case $\alpha = 1$ corresponds to concentration in position only,

$$\lim_\varepsilon W_\varepsilon\psi_{0,\varepsilon} = \delta_{x_0} \times (2\pi)^{-n}|\mathcal{F}\phi_0|^2(\cdot - p_0)\mathscr{L}^n,$$

and the case $\alpha = 0$ yields concentration in momentum only,

$$\lim_\varepsilon W_\varepsilon\psi_{0,\varepsilon} = |\phi_0(\cdot - x_0)|^2\mathscr{L}^n \times \delta_{p_0}.$$

Here and below, $(\mathcal{F}\phi_0)(p) = \int_{\mathbb{R}^n} e^{-ip\cdot x}\phi_0(x)\,dx$ denotes the (standard, not scaled) Fourier transform. But even in these cases there is considerable difficulty in the analysis of (1.14), since the difference quotients of U have a limit only at the $\mathscr{L}^n$-a.e. point.

For these initial conditions there is presumably no hope of achieving full convergence as $\varepsilon \to 0$ for *all* (x_0, p_0), since the limit problem is not well-posed. However, in the spirit of the theory of flows that we shall illustrate in the second part of the introduction, one may look at the family of solutions, indexed in the case of the initial conditions (1.17) by (x_0, p_0), as a whole. More generally, we are considering a family of solutions $\psi^\varepsilon_{t,w}$ to (1.1) indexed by a "random" parameter $w \in W$ running in a probability space $(W, \mathcal{F}, \mathbb{P})$, and achieve convergence "with probability 1," using the theory developed in the first part of the paper, under the no-concentration in mean assumptions

$$\sup_{\varepsilon>0}\sup_{t\in\mathbb{R}}\left\|\int_W W_\varepsilon\psi^\varepsilon_{t,w} * G^{(2n)}_\varepsilon\,d\mathbb{P}(w)\right\|_{L^\infty(\mathbb{R}^{2n})} < \infty, \tag{1.18}$$

$$\sup_{\varepsilon>0}\sup_{t\in\mathbb{R}}\left\|\int_W |\psi^\varepsilon_{t,w} * G^{(n)}_{\lambda\varepsilon^2}|^2\,d\mathbb{P}(w)\right\|_{L^\infty(\mathbb{R}^n)} \le C(\lambda) < \infty \quad \forall\lambda > 0. \tag{1.19}$$

Here $G^{(2n)}_\varepsilon$ is the Gaussian kernel in $\mathbb{R}^{2n}$ with variance $\varepsilon/2$. Under these assumptions and those on U given in Section 7.2, our full convergence result reads as follows:

$$\lim_{\varepsilon\downarrow 0}\int_W \sup_{t\in[-T,T]} d_{\mathcal{A}'}(W_\varepsilon\psi^\varepsilon_{t,w}, \boldsymbol{\mu}(t,\mu_w))d\mathbb{P}(w) = 0 \qquad \forall\, T > 0 \tag{1.20}$$

(here $d_{\mathcal{A}'}$ is a suitable bounded distance inducing the weak-$*$ topology in the unit ball of $\mathcal{A}'$; see (7.8)), where $\boldsymbol{\mu}(t,\mu_w)$ is the flow in the space of probability measures at time t starting from μ_w, and $\mu_w = \lim_\varepsilon W_\varepsilon\psi^\varepsilon_{0,w}$ depends only on the initial conditions. For instance, in the case of the initial conditions (1.17) with $\|\phi_0\|_2 = 1$, indexed by $w = (x_0, p_0)$, $\mu_w = \delta_w$, and $\boldsymbol{\mu}(t,\mu_w) = \delta_{\boldsymbol{X}(t,w)}$, where $\boldsymbol{X}(t,w)$ is the unique regular Lagrangian flow in $\mathbb{R}^{2n}$ induced by $(p, -\nabla U)$; see Theorem 6.2. So we may say that the flow of Wigner measures, thought of as elements of $\mathcal{A}'$, induced by the Schrödinger equation converges as $\varepsilon \to 0$ to the flow in $\mathscr{P}(\mathbb{R}^{2n}) \subset \mathcal{A}'$ induced by the Liouville equation provided the initial conditions ensure (1.18) and (1.19).

Of course, one can question conditions (1.18) and (1.19); we show in Section 8 that both are implied by the uniform operator inequality (here ρ^{ψ} is the orthogonal projection on ψ)

$$\frac{1}{\varepsilon^n}\int_W \rho^{\psi^{\varepsilon}_{t,w}}\, d\mathbb{P}(w) \le C\,\mathrm{Id} \quad \text{with } C \text{ independent of } t, \varepsilon. \tag{1.21}$$

In turn, this latter property is propagated in time (i.e., if the inequality holds at $t = 0$, it holds for all times), and it is satisfied by the semiclassical wave packets (1.17) when integration with respect to $\mathbb{P}$ corresponds to averaging the position and momentum parameters x_0 and p_0 (see Section 8). These facts indicate that the no-concentration in mean conditions are not only technically convenient, but somehow natural.

An alternative approach to the flow viewpoint advocated here for validating classical dynamics (1.11) from quantum dynamics (1.1) would be to work with deterministic initial data but restrict them to those giving rise to suitable bounds, in mean, on the projection operators $\rho^{\psi_{0,\varepsilon}}$. The problem of finding sufficient conditions to ensure these uniform bounds is studied in [17]. Another related research direction is a finer analysis of the behavior of solutions, in the spirit of [14, 15]. However, this analysis is presently possible only for very particular cases of eigenvalue crossings.

It is likely that our results can be applied to many more families of initial conditions, but this is not the goal of this paper. The proof of (1.20) relies on several a priori and fine estimates and on the theoretical tools described in the second part of the introduction and announced in [5]. In particular, we apply the stability properties (see Theorem 5.2) of the regular Lagrangian flow in $\mathscr{P}(\mathbb{R}^{2n})$ with respect to a reference measure $\boldsymbol{\nu}$ ($\boldsymbol{\nu}$-RLF in short; see Definition 3.7 and the motivation below), to the Husimi transforms of $\psi^{\varepsilon}_{t,w}$, namely $W_\varepsilon\psi^{\varepsilon}_{t,w} * G^{(2n)}_{\varepsilon}$. Indeed, (1.20) follows basically by the fact that weak-$*$ convergence in $\mathcal{A}'$ of the Wigner transforms is implied by weak convergence in $\mathscr{P}(\mathbb{R}^{2n})$ of the Husimi transforms; see Section 7.

We leave aside further extensions analogous to those considered in [24], namely:

- the convergence of density matrices ρ^{ε}, whose dynamics is described by $i\varepsilon\partial_t\rho^{\varepsilon} = [H_\varepsilon, \rho^{\varepsilon}]$; in this connection, see [17];
- the nonlinear case when $U = U_0 * \mu$, μ being the position density of ψ (i.e., $|\psi|^2$).

Let us now describe the "flow" viewpoint first in finite-dimensional spaces, where by now the theory is well understood. With $\boldsymbol{b}_t : \mathbb{R}^d \to \mathbb{R}^d$, $t \in [0, T]$, denoting the possibly time-dependent velocity field, the first basic idea is not to look for pointwise uniqueness statements, but rather to the family of solutions to the ODE as a whole. This leads to the concept of the flow map $\boldsymbol{X}(t, x)$ associated to $\boldsymbol{b}$, i.e., a map satisfying $\boldsymbol{X}(0,x) = x$ and $\boldsymbol{X}(t,x) = \gamma(t)$, where $\gamma(0) = x$ and

$$\dot{\gamma}(t) = \boldsymbol{b}_t(\gamma(t)) \quad \text{for } \mathscr{L}^1\text{-a.e. } t \in (0,T) \tag{1.22}$$

for $\mathscr{L}^d$-a.e. $x \in \mathbb{R}^d$. It is easily seen that this is not an invariant concept, under modification of $\boldsymbol{b}$ in negligible sets, while many applications of the theory to fluid dynamics (see, for instance, [22, 23]) and conservation laws need this invariance property. This leads to the concept of *regular Lagrangian flow*: one may ask that, for all $t \in [0,T]$, the image of the Lebesgue measure $\mathscr{L}^d$ under the flow map $x \mapsto \boldsymbol{X}(t,x)$ still be controlled by $\mathscr{L}^d$ (see Definition 3.1). It is not hard to show that, because of the additional regularity condition imposed on $\boldsymbol{X}$, this concept is indeed invariant under modifications of $\boldsymbol{b}$ in Lebesgue negligible sets (see Remark 3.8). Hence RLFs are appropriate to deal with vector fields belonging to Lebesgue L^p-spaces. On the other hand, since this regularity condition involves all trajectories $\boldsymbol{X}(\cdot,x)$ up to $\mathscr{L}^d$-negligible sets of initial data, the best we can hope for using this concept is existence and uniqueness of $\boldsymbol{X}(\cdot,x)$ up to $\mathscr{L}^d$-negligible sets. Intuitively, this can be viewed as existence and uniqueness "with probability 1" with respect to a reference measure on the space of initial data. Notice that already in the finite-dimensional theory different reference measures (e.g., Gaussian, see [4]) could be considered as well.

To establish such existence and uniqueness, one uses that the concept of flow is directly linked, via the theory of characteristics, to the transport equation

$$\frac{d}{ds} f(s,x) + \langle \boldsymbol{b}_s(x), \nabla_x f(s,x) \rangle = 0 \tag{1.23}$$

and to the continuity equation

$$\frac{d}{dt}\mu_t + \nabla \cdot (\boldsymbol{b}_t \mu_t) = 0. \tag{1.24}$$

The first equation has been exploited in [13] to transfer well-posedness results from the transport equation to the ODE, getting uniqueness of RLF (with respect to Lebesgue measure) in $\mathbb{R}^d$. This is possible because the flow maps $(s,x) \mapsto \boldsymbol{X}(t,s,x)$ (here we made also explicit the dependence on the initial time s, previously set to 0) solve (1.23) for all $t \in [0,T]$. In the present article, in analogy with the approach initiated in [1] (see also [16] for a stochastic counterpart of it, where (1.24) becomes the forward Kolmogorov equation), we prefer rather to deal with the continuity equation, which seems to be more natural in a probabilistic framework. The link between the ODE (1.22) and the continuity equation (1.24) can be made precise as follows: any positive finite measure $\boldsymbol{\eta}$ on initial values and paths, $\boldsymbol{\eta} \in \mathscr{P}(\mathbb{R}^d \times C([0,T];\mathbb{R}^d))$, concentrated on solutions (x,γ) to the ODE with initial condition $x = \gamma(0)$, gives rise to a (distributional) solution to (1.24), with μ_t given by the marginals of $\boldsymbol{\eta}$ at time t: indeed, (1.24) describes the evolution of a probability density under the action of the "velocity field" $\boldsymbol{b}$. We shall call these measures $\boldsymbol{\eta}$ *generalized* flows; see Definition 3.4.

These facts lead to the existence, the uniqueness (up to $\mathscr{L}^d$-negligible sets), and the stability of the RLF $\boldsymbol{X}(t,x)$ in $\mathbb{R}^d$ *provided* (1.24) is well-posed in $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$. Roughly speaking, this should be thought of as a regularity assumption on $\boldsymbol{b}$. See Remark 3.2 and Section 6 for explicit conditions on $\boldsymbol{b}$ ensuring well-posedness.

We shall extend all these results to flows on $\mathscr{P}(\mathbb{R}^d)$, the space of probability measures on $\mathbb{R}^d$. The heuristic idea is that (1.24) can be viewed as a (constant coefficients) ODE in the infinite-dimensional space $\mathscr{P}(\mathbb{R}^d)$ and that we can achieve uniqueness results for (1.24) for "almost every" measure initial condition. We need, however, a suitable reference measure on $\mathscr{P}(\mathbb{R}^d)$, which we shall denote by $\boldsymbol{\nu}$. Our theory works for many choices of $\boldsymbol{\nu}$ (in agreement with the fact that no canonical choice of $\boldsymbol{\nu}$ seems to exist) provided $\boldsymbol{\nu}$ satisfies the *regularity* condition

$$\int_{\mathscr{P}(\mathbb{R}^d)} \mu \, d\boldsymbol{\nu}(\mu) \le C \mathscr{L}^d,$$

see Definition 3.5. (See also Example 3.6 for some natural choices of regular measures $\boldsymbol{\nu}$.) Given $\boldsymbol{\nu}$ as reference measure, and assuming that (1.24) is well-posed in $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$, we prove existence, uniqueness (up to $\boldsymbol{\nu}$-negligible sets), and stability of the regular Lagrangian flow of measures $\boldsymbol{\mu}$. Since this assumption is precisely the one needed to have existence and uniqueness of the RLF $\boldsymbol{X}(t,x)$ in $\mathbb{R}^d$, it turns out that the RLF $\boldsymbol{\mu}(t,\mu)$ in $\mathscr{P}(\mathbb{R}^d)$ is given by

$$\boldsymbol{\mu}(t,\mu) = \int_{\mathbb{R}^d} \delta_{\boldsymbol{X}(t,x)} \, d\mu(x) \quad \forall t \in [0,T], \ \mu \in \mathscr{P}(\mathbb{R}^d), \tag{1.25}$$

which makes the existence part of our results rather easy whenever an underlying flow $\boldsymbol{X}$ in $\mathbb{R}^d$ exists. On the other hand, even in this situation, it turns out that uniqueness and stability results are much stronger when stated at the $\mathscr{P}(\mathbb{R}^d)$ level.

In our proofs, which follow by an infinite-dimensional adaptation of [1, 2], we also use the concept of generalized flow in $\mathscr{P}(\mathbb{R}^d)$, i.e., measures $\boldsymbol{\eta}$ on $\mathscr{P}(\mathbb{R}^d) \times C([0,T]; \mathscr{P}(\mathbb{R}^d))$ concentrated on initial data/solution pairs (μ, ω) to (1.24) with $\omega(0) = \mu$; see Definition 3.9.

Organization of the Paper

The paper consists of two main parts: the first one devoted to the above-mentioned extension of the theory of flows to the case when the state space is $\mathscr{P}(\mathbb{R}^d)$, and the second one focused on the specific application to semiclassical limits. After the illustration of the basic measure-theoretic notation and concepts in Section 2, in Section 3 we present the axiomatization of the theory of flows based on the continuity equation. Section 4 contains new existence and uniqueness results for flows in $\mathscr{P}(\mathbb{R}^d)$. The more abstract part of the paper ends in Section 5, where uniqueness is improved to stability with respect to families of approximate solutions to the continuity equation, such as those appearing in semiclassical limits.

In Section 6 we prove that, even in the presence of Coulomb singularities, when the interaction is repulsive only it is still possible to obtain uniqueness of solutions by a localization in (phase) space. In Section 7 we study solutions to (1.1), focusing in particular on estimates and convergence of the error term $\mathscr{E}_\varepsilon(U,\psi)$ in (1.14); its bilinear character allows us to deal separately with the Coulomb part U_s, which is treated using lemma 5.1 in [6], and the part U_b comprising the kinetic energy of the electrons and their interaction with electrons and nuclei. In Section 8 we provide new L^∞-estimates on the averaged Husimi transforms and show that they are implied by the uniform operator inequalities (1.21). In Section 9 we gather all previous results and prove the convergence of Wigner-Husimi transforms.

2 Notation and Preliminary Results

Let X be a Polish space (i.e., a separable topological space whose topology is induced by a complete distance). We shall denote by $\mathcal{B}(X)$ the σ-algebra of Borel sets of X, by $\mathscr{P}(X)$ the space of Borel probability measures on X, and by $\mathscr{M}(X)$ and $\mathscr{M}_+(X)$ the space of finite Borel and finite Borel nonnegative measures on X, respectively. For $A \in \mathcal{B}(X)$ and $\nu \in \mathscr{M}(X)$, we denote by $\nu \llcorner A \in \mathscr{M}(X)$ the restricted measure, namely $\nu \llcorner A(B) = \nu(A \cap B)$. Given $f : X \to Y$ Borel and $\mu \in \mathscr{M}(X)$, we denote by $f_\sharp\mu \in \mathscr{M}(Y)$ the pushforward measure on Y, i.e., $f_\sharp\mu(A) = \mu(f^{-1}(A))$ (if μ is a probability measure, $f_\sharp\mu$ is the law of f under μ), and we recall the basic integration rule

$$\int_Y \phi \, df_\sharp\mu = \int_X \phi \circ f \, d\mu \quad \text{for } \phi \text{ bounded and Borel.}$$

We denote by χ_A the characteristic function of a set A equal to 1 on A and equal to 0 on its complement. Balls in euclidean spaces will be denoted by $B_R(x_0)$ and by B_R if $x_0 = 0$.

We shall endow $\mathscr{P}(X)$ with the metrizable topology induced by the duality with $C_b(X)$, the space of continuous bounded functions on X: this makes $\mathscr{P}(X)$ itself a Polish space (see, e.g., [7, remark 5.1.1]), and we shall also consider measures $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(X))$.

Typically we shall use Greek letters to denote measures, boldface Greek letters to denote measures on the space of measures, and occasionally $d_{\mathscr{P}}$ for a bounded distance in $\mathscr{P}(X)$ inducing the weak topology induced by the duality with $C_b(X)$ (no specific choice of $d_{\mathscr{P}}$ will be relevant for us). We recall that weak convergence of μ_n to μ implies

$$\lim_{n\to\infty} \int_X f \, d\mu_n = \int_X f \, d\mu \tag{2.1}$$

for all f bounded Borel, with a μ-negligible discontinuity set.

Also, in the case $X = \mathbb{R}^d$, recall that a sequence $(\mu_n) \subset \mathscr{P}(\mathbb{R}^d)$ weakly converges to a probability measure μ in the duality with $C_b(\mathbb{R}^d)$ if and only if it converges in the duality with (a dense subspace of) $C_c(\mathbb{R}^d)$.

We shall consider the space $C([0,T];\mathscr{P}(\mathbb{R}^d))$, whose generic element will be denoted by ω, endowed with the sup norm; for this space we use the compact notation $\Omega_T(\mathscr{P}(\mathbb{R}^d))$. We also use e_t as a notation for the evaluation map at time t, so that $e_t(\omega) = \omega(t)$. Again, we shall consider measures $\boldsymbol{\eta} \in \mathscr{M}_+(\Omega_T(\mathscr{P}(\mathbb{R}^d)))$ and the basic criterion we shall use is the following:

PROPOSITION 2.1 (Tightness) *Let $(\boldsymbol{\eta}_n) \subset \mathscr{M}_+(\Omega_T(\mathscr{P}(\mathbb{R}^d)))$ be a bounded family satisfying the following*:

(i) *Space Tightness. For all $\varepsilon > 0$,*

$$\sup_n \boldsymbol{\eta}_n(\{\omega : \sup_{t\in[0,T]} \omega(t)(\mathbb{R}^d \setminus B_R) > \varepsilon\}) \to 0 \quad \text{as } R \to \infty.$$

(ii) *Time Tightness. For all $\phi \in C_c^\infty(\mathbb{R}^d)$, $n \geq 1$, the map $t \mapsto \int_{\mathbb{R}^d} \phi \, d\omega(t)$ is absolutely continuous in $[0,T]$ for $\boldsymbol{\eta}_n$-a.e. ω and*

$$\lim_{M\uparrow\infty} \sup_n \boldsymbol{\eta}_n\left(\left\{\omega : \int_0^T \left|\left(\int_{\mathbb{R}^d} \phi \, d\omega(t)\right)'\right| dt > M\right\}\right) = 0.$$

Then $(\boldsymbol{\eta}_n)$ is tight.

PROOF. We shall denote by $I_\phi : \Omega_T(\mathscr{P}(\mathbb{R}^d)) \to C([0,T])$ the time-dependent integral with respect to ϕ for all $\phi \in C_c^\infty(\mathbb{R}^d)$. Since the sets

$$\left\{ f \in W^{1,1}(0,T) : \sup |f| \leq C, \int_0^T |f'(t)| dt \leq M \right\}$$

are compact in $C([0,T])$, by assumption (ii) the sequence $((I_\phi)_\sharp \boldsymbol{\eta}_n)$ is tight in $\mathscr{M}_+(C([0,T]))$ for all $\phi \in C_c^\infty(\mathbb{R}^d)$. Hence, if we fix a countable dense set $(\phi_k) \subset C_c^\infty(\mathbb{R}^d)$ and $\varepsilon > 0$, we can find for $k \geq 1$ compact sets $K_k^\varepsilon \subset C([0,T])$ such that $\sup_n \boldsymbol{\eta}_n(\Omega_T(\mathscr{P}(\mathbb{R}^d)) \setminus I_{\phi_k}^{-1}(K_k^\varepsilon)) < \varepsilon 2^{-k}$. Thus, if K^ε denotes the intersection of all sets $I_{\phi_k}^{-1}(K_k^\varepsilon)$, we get

$$\sup_n \boldsymbol{\eta}_n(\Omega_T(\mathscr{P}(\mathbb{R}^d)) \setminus K^\varepsilon) < \varepsilon.$$

Analogously, we can build another compact set $L^\varepsilon \subset \Omega_T(\mathscr{P}(\mathbb{R}^d))$ by using assumption (i) such that $\sup_n \boldsymbol{\eta}_n(\Omega_T(\mathscr{P}(\mathbb{R}^d)) \setminus L^\varepsilon) < \varepsilon$ and, for all integers $k \geq 1$, there exists $R = R_k$ such that $\omega(t)(\mathbb{R}^d \setminus B_R) < 1/k$ for all $\omega \in L^\varepsilon$ and $t \in [0,T]$.

In order to conclude, it suffices to show that $K^\varepsilon \cap L^\varepsilon$ is compact in $\Omega_T(\mathscr{P}(\mathbb{R}^d))$: if $(\omega_p) \subset K^\varepsilon \cap L^\varepsilon$ we can use the inclusion in $I_{\phi_k}^{-1}(K_k^\varepsilon)$ and a diagonal argument to extract a subsequence $(\omega_{p(\ell)})$ such that $\int \phi_k \, d\omega_{p(\ell)}(t)$ has a limit for all $t \in [0,T]$ and all $k \geq 1$ and the limit is continuous in time. By the space tightness given by the inclusion $(\omega_p) \subset L^\varepsilon$, $\omega_{p(\ell)}(t)$ converges to $\omega(t)$ in $\mathscr{P}(\mathbb{R}^d)$ for all $t \in [0,T]$, and $t \mapsto \omega(t)$ is continuous. □

The next lemma is a refinement of [2, lemma 22] and [27, cor. 5.23], and allows us to obtain convergence in probability from weak convergence of the measures induced on the graphs.

LEMMA 2.2 *Let* $f_n : X \to Y$ *and* $f : X \to Y$ *be Borel maps,* $\nu_n, \nu \in \mathscr{P}(X)$, *and assume that* $(\mathrm{Id} \times f_n)_\sharp \nu_n$ *weakly converge to* $(\mathrm{Id} \times f)_\sharp \nu$ *in* $X \times Y$. *Assume in addition that we have the Skorokhod representations* $\nu_n = (i_n)_\sharp \mathbb{P}$, $\nu = i_\sharp \mathbb{P}$, *with* $(W, \mathcal{F}, \mathbb{P})$ *a probability measure space,* $i_n, i : W \to X$ *measurable, and* $i_n \to i$ $\mathbb{P}$*-almost everywhere. Then* $f_n \circ i_n \to f \circ i$ *in* $\mathbb{P}$*-probability.*

PROOF. Let d_Y denote the distance in Y. Up to replacing d_Y by $\min\{d_Y, 1\}$, with no loss of generality we can assume that the distance in Y does not exceed 1. Fix $\varepsilon > 0$ and $g \in C_b(X;Y)$ with $\int_X d_Y(g,f)d\nu \le \varepsilon^2$. We have that $\{d_Y(f_n \circ i_n, f \circ i) > 3\varepsilon\}$ is contained in

$$\{d_Y(f_n \circ i_n, g \circ i_n) > \varepsilon\} \cup \{d_Y(g \circ i_n, g \circ i) > \varepsilon\} \cup \{d_Y(g \circ i, f \circ i) > \varepsilon\}.$$

The second set has infinitesimal $\mathbb{P}$-probability, since g is continuous and $i_n \to i$ $\mathbb{P}$-a.e.; the third set, by the Markov inequality, has $\mathbb{P}$-probability less than ε; to estimate the $\mathbb{P}$-probability of the first set, we notice that

$$\mathbb{P}(\{d_Y(f_n \circ i_n, g \circ i_n) > \varepsilon\}) = \nu_n(\{d_Y(f_n, g) > \varepsilon\}) \le \frac{1}{\varepsilon} \int\limits_{X \times Y} \chi \, d(\mathrm{Id} \times f_n)_\sharp \nu_n$$

with $\chi(x,y) := d_Y(g(x), y)$. The weak convergence of $(\mathrm{Id} \times f_n)_\sharp \nu_n$ yields

$$\begin{aligned}\limsup_{n\to\infty} \mathbb{P}(\{d_Y(f_n \circ i_n, g \circ i_n) > \varepsilon\}) &\le \frac{1}{\varepsilon} \int\limits_{X \times Y} \chi \, d(\mathrm{Id} \times f)_\sharp \nu \\ &= \frac{1}{\varepsilon} \int\limits_X d_Y(g(x), f(x)) d\nu(x) \le \varepsilon.\end{aligned}$$

□

3 Continuity Equations and Flows

In this section we shall specify the basic assumptions on $\boldsymbol{b}$ used throughout this paper, and the conventions about (1.24) concerning locally bounded (respectively, measure-valued) solutions. We shall also collect the basic definitions of regular flows that we shall work with, recalling first those used when the state space is $\mathbb{R}^d$ and then extending these concepts to $\mathscr{P}(\mathbb{R}^d)$.

3.1 Continuity Equations

We consider a Borel vector field $\boldsymbol{b} : [0,T]\times\mathbb{R}^d \to \mathbb{R}^d$, and set $\boldsymbol{b}_t(\cdot) := \boldsymbol{b}(t,\cdot)$; we *shall not* work with the Lebesgue equivalence class of $\boldsymbol{b}$, although a posteriori our theory is independent of the choice of the representative (see Remark 3.8); this is important in view of the fact that (1.24) involves possibly singular measures. Also, we *shall not* make any integrability assumption on $\boldsymbol{b}$ besides $L^1_{\mathrm{loc}}([0,T]\times\mathbb{R}^d)$ (namely, the Lebesgue integral of $|\boldsymbol{b}|$ is finite on $[0,T]\times B_R$ for all $R>0$); the latter is needed in order to give a distributional sense to the functional version of (1.24), namely,

$$\frac{d}{dt}w_t + \nabla\cdot(\boldsymbol{b}_t w_t) = 0 \tag{3.1}$$

coupled with an initial condition $w_0 = \bar{w} \in L^\infty_{\mathrm{loc}}(\mathbb{R}^d)$, when w_t is locally bounded in space-time.

It is well-known and easy to check that any distributional solution $w(t,x) = w_t(x)$ to (3.1) with w_t locally bounded in $\mathbb{R}^d$ uniformly in time can be modified in an $\mathscr{L}^1$-negligible set of times in such a way that $t\mapsto w_t$ is continuous with respect to the duality with $C_c(\mathbb{R}^d)$, and well-defined limits exist at $t=0$, $t=T$ (see, for instance, [7, lemma 8.1.2] for a detailed proof). In particular, the initial condition $w_0=\bar{w}$ is then well-defined, and we shall always work with this weakly continuous representative.

In what follows, we shall say that the continuity equation (3.1) has uniqueness in the cone of functions $L^\infty_+([0,T];L^1\cap L^\infty(\mathbb{R}^d))$ if, for any $\bar{w}\in L^1\cap L^\infty(\mathbb{R}^d)$ nonnegative, there exists at most one nonnegative solution w_t to (3.1) in $L^\infty([0,T];L^1\cap L^\infty(\mathbb{R}^d))$ satisfying the condition

$$w_0 = \bar{w}. \tag{3.2}$$

Coming to measure-valued solutions to (1.24), we say that $t\in[0,T]\mapsto\mu_t\in\mathscr{M}_+(\mathbb{R}^d)$ solves (1.24) if $|\boldsymbol{b}|\in L^1_{\mathrm{loc}}((0,T)\times\mathbb{R}^d;\mu_t\,dt)$, the equation holds in the sense of distributions, and $t\mapsto\int\phi\,d\mu_t$ is continuous in $[0,T]$ for all $\phi\in C_c(\mathbb{R}^d)$.

3.2 Flows in $\mathbb{R}^d$

DEFINITION 3.1 (ν-RLF in $\mathbb{R}^d$) Let $\boldsymbol{X} : [0,T]\times\mathbb{R}^d\to\mathbb{R}^d$ and $\nu\in\mathscr{M}_+(\mathbb{R}^d)$ with $\nu\ll\mathscr{L}^d$ and of bounded density. We say that $\boldsymbol{X}$ is a ν-RLF in $\mathbb{R}^d$ relative to $\boldsymbol{b}\in L^1_{\mathrm{loc}}([0,T]\times\mathbb{R}^d;\mathbb{R}^d)$ if the following two conditions are fulfilled:

(i) for ν-a.e. x, the function $t\mapsto\boldsymbol{X}(t,x)$ is an absolutely continuous integral solution to the ODE (1.22) in $[0,T]$ with $\boldsymbol{X}(0,x)=x$;

(ii) $\boldsymbol{X}(t,\cdot)_\#\nu\le C\mathscr{L}^d$ for all $t\in[0,T]$ for some constant C independent of t.

Notice that, in view of condition (ii), the assumption of bounded density of ν is necessary for the existence of the ν-RLF, as $\boldsymbol{X}(0,\cdot)_\#\nu=\nu$.

In this context, since all admissible initial measures ν are bounded above by $C\mathscr{L}^d$, uniqueness of the ν-RLF can and will be understood in the following stronger sense: if f, $g \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ are nonnegative and $\boldsymbol{X}$ and $\boldsymbol{Y}$ are, respectively, an $f\mathscr{L}^d$-RLF and a $g\mathscr{L}^d$-RLF, then $\boldsymbol{X}(\cdot, x) = \boldsymbol{Y}(\cdot, x)$ for $\mathscr{L}^d$-a.e. $x \in \{f > 0\} \cap \{g > 0\}$.

Remark 3.2 (BV Vector Fields). We shall use in particular the fact that the ν-RLF exists for all $\nu \le C\mathscr{L}^d$ and is unique in the strong sense described above under the following assumptions on $\boldsymbol{b}$: $|\boldsymbol{b}|$ is uniformly bounded, $\boldsymbol{b}_t \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)$, and $\nabla \cdot \boldsymbol{b}_t = g_t \mathscr{L}^d \ll \mathscr{L}^d$ for $\mathscr{L}^1$-a.e. $t \in (0,T)$, with

$$\|g_t\|_{L^\infty(\mathbb{R}^d)} \in L^1(0,T), \quad |D\boldsymbol{b}_t|(B_R) \in L^1(0,T) \quad \text{for all } R > 0,$$

where $|D\boldsymbol{b}_t|$ denotes the total variation of the distributional derivative of $\boldsymbol{b}_t$. See [1, 2] and the paper [12] for Hamiltonian vector fields.

Remark 3.3 ($\mathscr{L}^d$-RLF). In all situations where the ν-RLF exists and is unique, one can also define by an exhaustion procedure an $\mathscr{L}^d$-RLF $\boldsymbol{X}$, uniquely determined (and well-defined) by the property

$$\boldsymbol{X}(\cdot, x) = \boldsymbol{X}^f(\cdot, x) \quad \mathscr{L}^d\text{-a.e. on } \{f > 0\}$$

for all $f \in L^\infty \cap L^1(\mathbb{R}^d)$ nonnegative, where $\boldsymbol{X}^f$ is the $f\mathscr{L}^d$-flow. Also, it turns out that if (3.1) has *backward* uniqueness, and if the constant C in Definition 3.1(ii) can be chosen independently of $\nu \le \mathscr{L}^d$, then $\boldsymbol{X}(t,\cdot)_\sharp \mathscr{L}^d \le C\mathscr{L}^d$. We don't prove this last statement here, since it will not be needed in the rest of the paper, and we mention this just for completeness.

In the proof of stability and uniqueness results, it is actually more convenient to consider a generalized concept of flow; see [2] for a more complete discussion. We denote the evaluation map $(x,\omega) \in \mathbb{R}^d \times C([0,T];\mathbb{R}^d) \mapsto \omega(t) \in \mathbb{R}^d$ again with e_t.

DEFINITION 3.4 (Generalized ν-RLF in $\mathbb{R}^d$) Let $\nu \in \mathscr{M}_+(\mathbb{R}^d)$ and $\boldsymbol{\eta} \in \mathscr{P}(\mathbb{R}^d \times C([0,T];\mathbb{R}^d))$. We say that $\boldsymbol{\eta}$ is a generalized ν-RLF in $\mathbb{R}^d$ relative to $\boldsymbol{b} \in L^1_{\mathrm{loc}}([0,T] \times \mathbb{R}^d;\mathbb{R}^d)$ if:

- (i) $(e_0)_\sharp \boldsymbol{\eta} = \nu$;
- (ii) $\boldsymbol{\eta}$ is concentrated on the set of pairs (x,γ), with γ an absolutely continuous solution to (1.22), and $\gamma(0) = x$;
- (iii) $(e_t)_\sharp \boldsymbol{\eta} \le C\mathscr{L}^d$ for all $t \in [0,T]$ for some constant C independent of t.

3.3 Flows in $\mathscr{P}(\mathbb{R}^d)$

Given a nonnegative σ-finite measure $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$, we denote by $\mathbb{E}\boldsymbol{\nu} \in \mathscr{M}_+(\mathbb{R}^d)$ its expectation, namely,

$$\int_{\mathbb{R}^d} \phi \, d\mathbb{E}\boldsymbol{\nu} = \int_{\mathscr{P}(\mathbb{R}^d)} \int_{\mathbb{R}^d} \phi \, d\mu \, d\boldsymbol{\nu}(\mu) \quad \text{for all } \phi \text{ bounded Borel.}$$

DEFINITION 3.5 (Regular Measures on $\mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$) Let $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$. We say that $\boldsymbol{\nu}$ is *regular* if $\mathbb{E}\boldsymbol{\nu} \le C\mathscr{L}^d$ for some constant C.

Example 3.6.

(1) The first standard example of a regular measure $\boldsymbol{\nu}$ is the law under $\rho\mathscr{L}^d$ of the map $x \mapsto \delta_x$, with $\rho \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ nonnegative. Actually, one can even consider the law under $\mathscr{L}^d$, and in this case $\boldsymbol{\nu}$ would be σ-finite instead of a finite nonnegative measure.

(2) If $d = 2n$ and $z = (x, p) \in \mathbb{R}^n \times \mathbb{R}^n$ (this factorization corresponds for instance to flows in a phase space), one may consider the law under $\rho\mathscr{L}^n$ of the map $x \mapsto \delta_x \times \gamma$, with $\rho \in L^1(\mathbb{R}^n_x) \cap L^\infty(\mathbb{R}^n_x)$ nonnegative and $\gamma \in \mathscr{P}(\mathbb{R}^n_p)$ with $\gamma \le C\mathscr{L}^n$; one can also choose γ dependent on x, provided $x \mapsto \gamma_x$ is measurable and $\gamma_x \le C\mathscr{L}^n$ for some constant C independent of x.

(3) We also conjecture that the *entropic* measures built in [26, 28] are regular; see also the references therein for more examples of "natural" reference measures on the space of measures.

As we explained in the introduction, Definition 3.1 has a natural (but not perfect) transposition to flows in $\mathscr{P}(\mathbb{R}^d)$:

DEFINITION 3.7 ($\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$) Let $\boldsymbol{\mu} : [0, T] \times \mathscr{P}(\mathbb{R}^d) \to \mathscr{P}(\mathbb{R}^d)$ and $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$. We say that $\boldsymbol{\mu}$ is a $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$ relative to $\boldsymbol{b} \in L^1_{\text{loc}}([0, T] \times \mathbb{R}^d; \mathbb{R}^d)$ if

(i) for $\boldsymbol{\nu}$-a.e. μ, $t \mapsto \mu_t := \boldsymbol{\mu}(t, \mu)$ is (weakly) continuous from $[0, T]$ to $\mathscr{P}(\mathbb{R}^d)$ with $\boldsymbol{\mu}(0, \mu) = \mu$, and μ_t solves (1.24) in the sense of distributions;

(ii) $\mathbb{E}(\boldsymbol{\mu}(t, \cdot)_\sharp \boldsymbol{\nu}) \le C\mathscr{L}^d$ for all $t \in [0, T]$ for some constant C independent of t.

Notice that no $\boldsymbol{\nu}$-RLF can exist if $\boldsymbol{\nu}$ is not regular, as $\boldsymbol{\mu}(0, \cdot)_\sharp \boldsymbol{\nu} = \boldsymbol{\nu}$. Notice also that condition (ii) is in some sense weaker than $\boldsymbol{\mu}(t, \cdot)_\sharp \boldsymbol{\nu} \le C\boldsymbol{\nu}$ (which would be the analogue of (ii) in Definition 3.1 if we were allowed to choose $\nu = \mathscr{L}^d$; see also Remark 3.3), but it is sufficient for our purposes. As a matter of fact, because of infinite dimensionality, the requirement of quasi-invariance of $\boldsymbol{\nu}$ under the action of the flow $\boldsymbol{\mu}$ (namely, the condition $\boldsymbol{\mu}(t, \cdot)_\sharp \boldsymbol{\nu} \ll \boldsymbol{\nu}$) would be a quite strong condition: for instance, if the state space is a separable Banach space V, the reference measure γ is a nondegenerate Gaussian measure, and $\boldsymbol{b}(t, x) = v$, then $\boldsymbol{X}(t, x) = x + tv$, and the quasi-invariance occurs only if v belongs to the Cameron-Martin subspace H of V, a dense but γ-negligible subspace. In our framework, Example 3.6(2) provides a natural measure $\boldsymbol{\nu}$ that is not quasi-invariant, because its support is not invariant, under the flow: to realize that quasi-invariance may fail, it suffices to choose autonomous vector fields of the form $\boldsymbol{b}(x, p) := (p, -\nabla U(x))$.

Remark 3.8 (Invariance of $\boldsymbol{\nu}$-RLF). Assume that $\boldsymbol{\mu}(t, \mu)$ is a $\boldsymbol{\nu}$-RLF relative to $\boldsymbol{b}$ and $\tilde{\boldsymbol{b}}$ is a modification of $\boldsymbol{b}$, i.e., for $\mathscr{L}^1$-a.e. $t \in (0, T)$ the set $N_t := \{\boldsymbol{b}_t \ne \tilde{\boldsymbol{b}}_t\}$ is $\mathscr{L}^d$-negligible. Then, because of condition (ii) we know that, for all $t \in (0, T)$,

$\boldsymbol{\mu}(t,\mu)(N_t) = 0$ for $\boldsymbol{\nu}$-a.e. μ. By Fubini's theorem, we obtain that, for $\boldsymbol{\nu}$-a.e. μ, the set of times t such that $\boldsymbol{\mu}(t,\mu)(N_t) > 0$ is $\mathscr{L}^1$-negligible in $(0,T)$. As a consequence $t \mapsto \boldsymbol{\mu}(t,\mu)$ is a solution to (1.24) with $\tilde{\boldsymbol{b}}_t$ in place of $\boldsymbol{b}_t$, and $\boldsymbol{\mu}$ is a $\boldsymbol{\nu}$-RLF relative to $\tilde{\boldsymbol{b}}$ as well.

In the next definition, as in Definition 3.4, we are going to consider measures on $\mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d))$, the first factor being a convenient label for the initial position of the path (an equivalent description could be given using just measures on $\Omega_T(\mathscr{P}(\mathbb{R}^d))$, at the price of a heavier use of conditional probabilities; see [2, remark 11] for a more precise discussion). We keep using the notation e_t for the evaluation map, so that $e_t(\mu,\omega) = \omega(t)$.

DEFINITION 3.9 (Generalized $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$) Let $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$ and $\boldsymbol{\eta} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d)))$. We say that $\boldsymbol{\eta}$ is a generalized $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$ relative to $\boldsymbol{b} \in L^1_{\mathrm{loc}}([0,T] \times \mathbb{R}^d; \mathbb{R}^d)$ if:

- (i) $(e_0)_\sharp \boldsymbol{\eta} = \boldsymbol{\nu}$;
- (ii) $\boldsymbol{\eta}$ is concentrated on the set of pairs (μ,ω), with ω solving (1.24), $\omega(0) = \mu$;
- (iii) $\mathbb{E}((e_t)_\sharp \boldsymbol{\eta}) \le C\mathscr{L}^d$ for all $t \in [0,T]$ for some constant C independent of t.

Again, by conditions (i) and (iii), no generalized $\boldsymbol{\nu}$-RLF can exist if $\boldsymbol{\nu}$ is not regular. Of course any $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}$ induces a generalized $\boldsymbol{\nu}$-RLF $\boldsymbol{\eta}$: it suffices to define

$$\boldsymbol{\eta} := (\Psi_{\boldsymbol{\mu}})_\sharp \boldsymbol{\nu}, \tag{3.3}$$

where

$$\Psi_{\boldsymbol{\mu}} : \mathscr{P}(\mathbb{R}^d) \to \mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d)), \quad \Psi_{\boldsymbol{\mu}}(\mu) := (\mu, \boldsymbol{\mu}(\cdot,\mu)). \tag{3.4}$$

It turns out that existence results are stronger at the RLF level, while results concerning uniqueness are stronger at the generalized RLF level.

The transfer mechanisms between generalized and classical flows, and between flows in $\mathscr{P}(\mathbb{R}^d)$ and flows in $\mathbb{R}^d$, are illustrated by the next proposition.

PROPOSITION 3.10 *Let $\boldsymbol{\eta}$ be a generalized $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$ relative to $\boldsymbol{b}$. Then*:

- (1) *$\mathbb{E}\boldsymbol{\eta}$ is a generalized $\mathbb{E}\boldsymbol{\nu}$-RLF in $\mathbb{R}^d$ relative to $\boldsymbol{b}$*;
- (2) *the measures $\mu_t := \mathbb{E}((e_t)_\sharp \boldsymbol{\eta}) = (e_t)_\sharp \mathbb{E}\boldsymbol{\eta} \in \mathscr{M}_+(\mathbb{R}^d)$ satisfy* (1.24).

In addition, $\mu_t = w_t \mathscr{L}^d$ with $w \in L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$.

PROOF. Statement (i) is easy to prove, since the continuity equation is linear. Statement (ii), namely that (single) time marginals of generalized flows in $\mathbb{R}^d$ solve (1.24), is proved in detail in [2, p. 8]. The final statement follows by the regularity condition on $\boldsymbol{\eta}$. □

4 Existence and Uniqueness of Regular Lagrangian Flows

In this section we recall the main existence and uniqueness results of the ν-RLF in $\mathbb{R}^d$, and see their extensions to $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$. It turns out that existence and uniqueness of solutions to (3.1) in $L^\infty_+([0,T];L^1 \cap L^\infty(\mathbb{R}^d))$ yields existence and uniqueness of the ν-RLF, and existence of this flow implies existence of the $\boldsymbol{\nu}$-RLF when $\boldsymbol{\nu}$ is regular. Also, the (apparently stronger) uniqueness of the $\boldsymbol{\nu}$-RLF is still implied by the uniqueness of solutions to (3.1) in $L^\infty_+([0,T];L^1 \cap L^\infty(\mathbb{R}^d))$.

The following result is proved in [2, theorem 19] for the part concerning existence and in [2, theorem 16, remark 17] for the part concerning uniqueness.

THEOREM 4.1 (Existence and Uniqueness of ν-RLF in $\mathbb{R}^d$) *Assume that* (3.1) *has existence and uniqueness in* $L^\infty_+([0,T];L^1 \cap L^\infty(\mathbb{R}^d))$. *Then, for all* $\nu \in \mathscr{M}(\mathbb{R}^d)$ *with* $\nu \ll \mathscr{L}^d$ *and of bounded density, the* ν*-RLF in* $\mathbb{R}^d$ *exists and is unique.*

Now we can easily show that existence of the ν-RLF implies existence of the $\boldsymbol{\nu}$-RLF, by a superposition principle. However, one might speculate that, for very rough vector fields, a $\boldsymbol{\nu}$-RLF might exist in $\mathscr{P}(\mathbb{R}^d)$, not induced by any ν-RLF in $\mathbb{R}^d$.

THEOREM 4.2 (Existence of $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$) *Let* $\nu \in \mathscr{M}(\mathbb{R}^d)$ *with* $\nu \ll \mathscr{L}^d$ *and of bounded density, and assume that a* ν*-RLF* $\boldsymbol{X}$ *in* $\mathbb{R}^d$ *exists. Then, for all* $\boldsymbol{\nu} \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$ *with* $\mathbb{E}\boldsymbol{\nu} = \nu$, *a* $\boldsymbol{\nu}$*-RLF* $\boldsymbol{\mu}$ *in* $\mathscr{P}(\mathbb{R}^d)$ *exists, and it is given by*

$$\boldsymbol{\mu}(t,\mu) := \int_{\mathbb{R}^d} \delta_{\boldsymbol{X}(t,x)} d\mu(x). \tag{4.1}$$

PROOF. The first part of property (i) in Definition 3.7 is obviously satisfied, since the fact that $t \mapsto \boldsymbol{X}(t,x)$ solves the ODE for some x corresponds to the fact that $t \mapsto \delta_{\boldsymbol{X}(t,x)}$ solves (1.24). On the other hand, since $\boldsymbol{\nu}$ is regular and $\boldsymbol{X}$ is an RLF, we know that $\boldsymbol{X}(\cdot,x)$ solves the ODE for $\mathbb{E}\boldsymbol{\nu}$-a.e. x; it follows that, for $\boldsymbol{\nu}$-a.e. μ, $\boldsymbol{X}(\cdot,x)$ solves the ODE for μ-a.e. x; hence $\boldsymbol{\mu}(t,\mu)$ solves (1.24) for $\boldsymbol{\nu}$-a.e. μ. This proves (i).

Property (ii) follows by

$$\begin{aligned}
\int_{\mathbb{R}^d} \phi(x) d\mathbb{E}(\boldsymbol{\mu}(t,\cdot)_\sharp \boldsymbol{\nu})(x) &= \int_{\mathscr{P}(\mathbb{R}^d)} \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}(t,\mu) d\boldsymbol{\nu}(\mu) \\
&= \int_{\mathscr{P}(\mathbb{R}^d)} \int_{\mathbb{R}^d} \phi(\boldsymbol{X}(t,x)) d\mu(x) d\boldsymbol{\nu}(\mu) \\
&= \int_{\mathbb{R}^d} \phi(\boldsymbol{X}(t,x)) d\nu(x) \le CL \int_{\mathbb{R}^d} \phi(z) dz
\end{aligned}$$

where C is the same constant as in Definition 3.1(ii) and L satisfies $\nu \le L\mathscr{L}^d$. □

The following lemma (a slight refinement of theorem 5.1 in [1] and lemma 4.6 in [4]) provides a simple characterization of Dirac masses for measures that are on $C_w([0,T];E)$ and for families of measures on E. Here E is a closed, convex, and bounded subset of the dual of a separable Banach space, endowed with a distance d_E inducing the weak-$*$ topology, so that (E, d_E) is a compact metric space; $C_w([0,T];E)$ denotes the space of continuous maps with values in (E, d_E), endowed with sup norm (so that these maps are continuous with respect to the weak-$*$ topology). We shall apply this result in the proof of Theorem 4.4 with

$$E := \{\mu \in \mathscr{M}(\mathbb{R}^d) : |\mu|(\mathbb{R}^d) \leq 1\} \supset \mathscr{P}(\mathbb{R}^d), \tag{4.2}$$

thought of as a subset of $(C_0(\mathbb{R}^d))^*$, where $C_0(\mathbb{R}^d)$ denotes the set of continuous functions vanishing at infinity (i.e., the closure of $C_c(\mathbb{R}^d)$ with respect to the uniform convergence).

LEMMA 4.3 *Let $E \subset G^*$, with G a separable Banach space, be closed, convex, and bounded, and let $\boldsymbol{\sigma}$ be a positive finite measure on $C_w([0,T];E)$. Then $\boldsymbol{\sigma}$ is a Dirac mass if and only if $(e_t)_\sharp\boldsymbol{\sigma}$ is a Dirac mass for all $t \in \mathbb{Q} \cap [0,T]$. If $(F, \mathcal{F}, \lambda)$ is a measure space, and a Borel family $\{\nu_z\}_{z\in F}$ of probability measures on E (i.e., $z \mapsto \nu_z(A)$ is $\mathcal{F}$-measurable in F for all $A \subset E$ Borel) is given, then ν_z are Dirac masses for λ-a.e. $z \in F$ if and only if for all y in a dense subset of G and all c in a dense subset of $\mathbb{R}$ there holds*

$$\nu_z(\{x \in E : \langle x, y\rangle \leq c\})\nu_z(\{x \in E : \langle x, y\rangle > c\}) = 0 \quad \text{for } \lambda\text{-a.e. } z \in F. \tag{4.3}$$

PROOF. The first statement is a direct consequence of the fact that all elements of $C_w([0,T];E)$ are weak-$*$ continuous maps, which are uniquely determined on $\mathbb{Q} \cap [0,T]$. In order to prove the second statement, let us consider the sets $A_{ij} := \{x \in E : \langle x, y_i\rangle \leq c_j\}$, where y_i vary in a countable dense set of G and c_j vary in a dense subset of $\mathbb{R}$. By (4.3) we obtain a λ-negligible set $N_{ij} \in \mathcal{F}$ satisfying $\nu_z(A_{ij})\nu_z(E \setminus A_{ij}) = 0$ for all $z \in F \setminus N_{ij}$. As a consequence, each measure ν_z, as z varies in $F \setminus N_{ij}$, is either concentrated on A_{ij} or on its complement. For $z \in F \setminus \bigcup_j N_{ij}$ it follows that the function $x \mapsto \langle x, y_i\rangle$ is equivalent to a constant up to ν_z-negligible sets. Since the functions $x \mapsto \langle x, y_i\rangle$ separate points of E, ν_z is a Dirac mass for all $z \in F \setminus \bigcup_{i,j} N_{ij}$, as desired. □

The next result shows that uniqueness of (1.24) in $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$ and existence of a generalized $\boldsymbol{\nu}$-RLF imply existence of the $\boldsymbol{\nu}$-RLF and uniqueness of both, the $\boldsymbol{\nu}$-RLF and the generalized $\boldsymbol{\nu}$-RLF.

THEOREM 4.4 (Existence and Uniqueness of the $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$) *Assume that* (3.1) *has uniqueness in $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$. If a generalized $\boldsymbol{\nu}$-RLF $\boldsymbol{\eta}$ in $\mathscr{P}(\mathbb{R}^d)$ exists, then the $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}$ in $\mathscr{P}(\mathbb{R}^d)$ exists. Moreover, they are both unique and related as in* (3.3) *and* (3.4)*.*

PROOF. We fix a generalized $\boldsymbol{\nu}$-RLF $\boldsymbol{\eta}$ and show first that $\boldsymbol{\eta}$ is induced by a $\boldsymbol{\nu}$-RLF (this will prove in particular the existence of the $\boldsymbol{\nu}$-RLF). To this end, denoting by $\pi : \mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d)) \to \mathscr{P}(\mathbb{R}^d)$ the projection on the first factor, we define by

$$\boldsymbol{\eta}_\mu := \mathbb{E}(\boldsymbol{\eta}|\pi = \mu) \in \mathscr{P}(\Omega_T(\mathscr{P}(\mathbb{R}^d)))$$

the induced conditional probabilities, so that $d\boldsymbol{\eta}(\mu, \omega) = d\boldsymbol{\eta}_\mu(\omega) d\boldsymbol{\nu}(\mu)$. Taking into account the first statement in Lemma 4.3, it suffices to show that, for $\bar{t} \in \mathbb{Q} \cap [0, T]$ fixed, the measures

$$\theta_\mu := \mathbb{E}((e_{\bar{t}})_\sharp \boldsymbol{\eta}|\omega(0) = \mu) = (e_{\bar{t}})_\sharp \boldsymbol{\eta}_\mu \in \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d))$$

are Dirac masses for $\boldsymbol{\nu}$-a.e. $\mu \in \mathscr{P}(\mathbb{R}^d)$. Still using Lemma 4.3, we will check the validity of (4.3) with $\lambda = \boldsymbol{\nu}$. Since $\theta_\mu = \delta_\mu$ when $\bar{t} = 0$, we shall assume that $\bar{t} > 0$.

Let us argue by contradiction, assuming the existence of $L \in \mathcal{B}(\mathscr{P}(\mathbb{R}^d))$ with $\boldsymbol{\nu}(L) > 0$, $\phi \in C_0(\mathbb{R}^d)$, and $c \in \mathbb{R}$ such that both $\theta_\mu(A)$ and $\theta_\mu(\mathscr{P}(\mathbb{R}^d) \setminus A)$ are strictly positive for all $\mu \in L$, with

$$A := \left\{\rho \in \mathscr{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \phi \, d\rho \le c\right\}.$$

We will get a contradiction under the assumption that equation (3.1) has uniqueness in $L^\infty_+([0, T]; L^1 \cap L^\infty(\mathbb{R}^d))$ by constructing two distinct nonnegative solutions of the continuity equation with the same initial condition $\bar{w} \in L^1 \cap L^\infty(\mathbb{R}^d)$. With no loss of generality, possibly passing to a smaller set L still with positive $\boldsymbol{\nu}$-measure, we can assume that the quotient $g(\mu) := \theta_\mu(A)/\theta_\mu(\mathscr{P}(\mathbb{R}^d) \setminus A)$ is uniformly bounded in L. Let $\Omega_1 \subset \Omega_T(\mathscr{P}(\mathbb{R}^d))$ be the set of trajectories ω that belong to A at time $\bar{t}$, and let Ω_2 be its complement; we can define positive finite measures $\boldsymbol{\eta}^i$, $i = 1, 2$, in $\mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d))$ by

$$d\boldsymbol{\eta}^1(\mu, \omega) := d(\chi_{\Omega_1}\boldsymbol{\eta}_\mu)(\omega) d(\chi_L \boldsymbol{\nu})(\mu),$$
$$d\boldsymbol{\eta}^2(\mu, \omega) := d(\chi_{\Omega_2}\boldsymbol{\eta}_\mu)(\omega) d(\chi_L g \boldsymbol{\nu})(\mu).$$

By Proposition 3.10, both $\boldsymbol{\eta}^1$ and $\boldsymbol{\eta}^2$ induce solutions w^1_t and w^2_t to the continuity equation, which are uniformly bounded (just by comparison with the one induced by $\boldsymbol{\eta}$) in space and time. Moreover, since

$$(e_0)_\sharp \boldsymbol{\eta}^1 = \theta_\mu(A)\chi_L(\mu)\boldsymbol{\nu}$$

and analogously

$$(e_0)_\sharp \boldsymbol{\eta}^2 = \theta_\mu(\mathscr{P}(\mathbb{R}^d) \setminus A)\chi_L(\mu) g(\mu)\boldsymbol{\nu},$$

our definition of g gives that $(e_0)_\sharp \boldsymbol{\eta}^1 = (e_0)_\sharp \boldsymbol{\eta}^2$. Hence, both solutions w^1_t and w^2_t start from the same initial condition $\bar{w}(x)$, namely the density of $\mathbb{E}(\theta_\mu(A)\chi_L(\mu)\boldsymbol{\nu})$

with respect to $\mathscr{L}^d$. On the other hand, it turns out that

$$\int_{\mathbb{R}^d} \phi w_t^1 \, dx = \int_L \int_{\Omega_1} \int_{\mathbb{R}^d} \phi \, d\omega(\overline{t}) d\boldsymbol{\eta}_\mu(\omega) d\boldsymbol{\nu}(\mu)$$

$$= \int_L \int_{\Omega_T(\mathscr{P}(\mathbb{R}^d))} \chi_A(\omega(\overline{t})) \int_{\mathbb{R}^d} \phi \, d\omega(\overline{t}) d\boldsymbol{\eta}_\mu(\omega) d\boldsymbol{\nu}(\mu)$$

$$= \int_L \int_A \int_{\mathbb{R}^d} \phi \, d\rho \, d\theta_\mu(\rho) d\boldsymbol{\nu}(\mu) \leq c \int_L \theta_\mu(A) d\boldsymbol{\nu}(\mu).$$

Analogously, we have

$$\int_{\mathbb{R}^d} \phi w_t^2 \, dx > c \int_L \theta_\mu(\mathscr{P}(\mathbb{R}^d) \setminus A) g(\mu) d\boldsymbol{\nu}(\mu) = c \int_L \theta_\mu(A) d\boldsymbol{\nu}(\mu).$$

Therefore $w_t^1 \neq w_t^2$ and uniqueness of the continuity equation is violated.

Now we can prove uniqueness of the generalized ν-RLF and of the generalized $\boldsymbol{\nu}$-RLF: if $\boldsymbol{\sigma}$ is any other generalized $\boldsymbol{\nu}$-RLF, we know $\boldsymbol{\sigma}$ is induced by a $\boldsymbol{\nu}$-RLF; hence for $\boldsymbol{\nu}$-a.e. μ the measures $\mathbb{E}(\boldsymbol{\sigma} | \omega(0) = \mu)$ are also Dirac masses; but since the property of being a generalized flow is stable under convex combinations, the measures (corresponding to the generalized $\boldsymbol{\nu}$-RLF $(\boldsymbol{\eta} + \boldsymbol{\sigma})/2$)

$$\frac{1}{2} \mathbb{E}(\boldsymbol{\eta} | \omega(0) = \mu) + \frac{1}{2} \mathbb{E}(\boldsymbol{\sigma} | \omega(0) = \mu) = \mathbb{E}\left(\frac{\boldsymbol{\eta} + \boldsymbol{\sigma}}{2} | \omega(0) = \mu \right)$$

must also be Dirac masses for $\boldsymbol{\nu}$-a.e. μ. This can happen only if $\mathbb{E}(\boldsymbol{\eta} | \omega(0) = \mu) = \mathbb{E}(\boldsymbol{\sigma} | \omega(0) = \mu)$ for $\boldsymbol{\nu}$-a.e. μ, hence $\boldsymbol{\sigma} = \boldsymbol{\eta}$. Finally, since distinct $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}$ and $\boldsymbol{\mu}'$ induce distinct generalized $\boldsymbol{\nu}$-RLF $\boldsymbol{\eta}$ and $\boldsymbol{\eta}'$, uniqueness is also proved for $\boldsymbol{\nu}$-RLF. □

5 The Stability of $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$

In the statement of the stability result we shall consider varying measures $\boldsymbol{\nu}_n \in \mathscr{P}(\mathscr{P}(\mathbb{R}^d))$, $n \geq 1$, and a limit measure $\boldsymbol{\nu}$. (The assumption that all $\boldsymbol{\nu}_n$ are probability measures is made in order to avoid technicalities that would obscure the main ideas behind our stability result, and one can always reduce to this case by renormalizing the measures. Moreover, in the applications we have in mind, our measures $\boldsymbol{\nu}_n$ will always have unitary total mass.) We shall assume that the $\boldsymbol{\nu}_n$ are generated as $(i_n)_\sharp \mathbb{P}$, where $(W, \mathcal{F}, \mathbb{P})$ is a probability measure space and $i_n : W \to \mathscr{P}(\mathbb{R}^d)$ are measurable; accordingly, we shall also assume that $\boldsymbol{\nu} = i_\sharp \mathbb{P}$, with $i_n \to i$ $\mathbb{P}$-a.e. These assumptions are satisfied in the applications we have in mind, and in any case Skorokhod's theorem (see [11, vol. II, sec. 8.5]) could be used to show that weak convergence of $\boldsymbol{\nu}_n$ to $\boldsymbol{\nu}$ always implies this sort of representation, even with $W = [0, 1]$ endowed with the standard measure structure, for suitable i_n and i.

Many formulations of the stability result are indeed possible, and we have chosen a specific one for the application we have in mind. Henceforth we fix an autonomous vector field $\boldsymbol{b} : \mathbb{R}^d \to \mathbb{R}^d$ satisfying the following regularity conditions:

(a) $d = 2n$ and $\boldsymbol{b}(x, p) = (p, \boldsymbol{c}(x))$, $(x, p) \in \mathbb{R}^d$, $\boldsymbol{c} : \mathbb{R}^n \to \mathbb{R}^n$ Borel and locally integrable;

(b) there exists a closed $\mathscr{L}^n$-negligible set S such that $\boldsymbol{c}$ is locally bounded on $\mathbb{R}^n \setminus S$;

(c) the discontinuity set Σ of $\boldsymbol{c}$ is $\mathscr{L}^n$-negligible.

LEMMA 5.1 *Let $S \subset \mathbb{R}^n$ closed, and assume that $\boldsymbol{b}$ is representable as in* (a) *above. Let $\mu_t : [0,T] \to \mathscr{P}(\mathbb{R}^d)$ solve* (1.24) *in the sense of distributions in $(\mathbb{R}^n \setminus S) \times \mathbb{R}^n$ and assume that*

$$\int_0^T \int_{B_R} \frac{1}{\operatorname{dist}^\beta(x,S)}\, d\mu_t(x,p)dt < \infty \quad \forall R > 0$$

for some $\beta > 1$ (with the convention $1/0 = +\infty$). Then (1.24) *holds in the sense of distributions in $\mathbb{R}^d$.*

PROOF. First of all, the assumption implies that $\mu_t(S \times \mathbb{R}^n) = 0$ for $\mathscr{L}^1$-a.e. $t \in (0,T)$. The proof of the global validity of the continuity equation uses the classical argument of removing the singularity by multiplying any test function $\phi \in C_c^\infty(\mathbb{R}^d)$ by χ_k, where $\chi_k(x) = \chi(k \operatorname{dist}(x,S))$ and χ is a smooth cutoff function equal to 0 on $[0,1]$ and equal to 1 on $[2,+\infty)$, with $0 \le \chi' \le 2$. If we use $\phi\chi_k$ as a test function, since χ_k depends on x only, we can use the particular structure (a) of $\boldsymbol{b}$ to write the term depending on the derivatives of χ_k as

$$k \int_0^T \int_{\mathbb{R}^d} \phi \chi'(k \operatorname{dist}(x,S)) \langle p, \nabla \operatorname{dist}(x,S)\rangle d\mu_t(x,p)dt.$$

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

$$2 \max_K |p\phi| \int_0^T \int_{\{x\in K: k \operatorname{dist}(x,S)\le 2\}} k\, d\mu_t(x,p)dt \le \frac{2^{\beta+1} \max_K |p\phi|}{k^{\beta-1}} \int_0^T \int_K \frac{1}{\operatorname{dist}^\beta(x,S)}\, d\mu_t(x,p)dt$$

and as $\beta > 1$ the right-hand side is infinitesimal since $k \to \infty$. □

The following stability result is adapted to the application we have in mind: we shall apply it to the case when $\boldsymbol{\mu}_n(t,\mu)$ are Husimi transforms of wave functions.

THEOREM 5.2 (Stability of $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^d)$) *Let i_n and i be as above and let $\boldsymbol{\mu}_n : [0,T] \times i_n(W) \to \mathscr{P}(\mathbb{R}^d)$ satisfy $\boldsymbol{\mu}_n(0, i_n(w)) = i_n(w)$ and the following conditions*:

(i) *Asymptotic Regularity.*

$$\limsup_{n\to\infty} \int_W \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w)) d\mathbb{P}(w) \le C \int_{\mathbb{R}^d} \phi \, dx$$

for all $\phi \in C_c(\mathbb{R}^d)$ *nonnegative for* C *independent of* t *and* ϕ.

(ii) *Uniform Decay Away from the Singularity. For some* $\beta > 1$

$$\sup_{\delta>0} \limsup_{n\to\infty} \int_W \int_0^T \int_{B_R} \frac{1}{\operatorname{dist}^\beta(x, S) + \delta} \, d\boldsymbol{\mu}_n(t, i_n(w)) dt \, d\mathbb{P}(w) < \infty \quad \forall R > 0. \tag{5.1}$$

(iii) *Space Tightness. For all* $\delta > 0$,

$$\mathbb{P}(\{w \in W : \sup_{t\in[0,T]} \boldsymbol{\mu}_n(t, i_n(w))(\mathbb{R}^d \setminus B_R) > \delta\}) \to 0$$

as $R \to \infty$ *uniformly in* n.

(iv) *Time Tightness. For* $\mathbb{P}$*-a.e.* $w \in W$, *for all* $n \ge 1$, *and* $\phi \in C_c^\infty(\mathbb{R}^d)$, $t \mapsto \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w))$ *is absolutely continuous in* $[0, T]$ *and, uniformly in* n,

$$\lim_{M\uparrow\infty} \mathbb{P}\left(\left\{w \in W : \int_0^T \left| \left(\int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w)) \right)' \right| dt > M \right\}\right) = 0.$$

(v) *Limit Continuity Equation.*

$$\lim_{n\to\infty} \int_W \left| \int_0^T \left[\varphi'(t) \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w)) + \varphi(t) \int_{\mathbb{R}^d} \langle \boldsymbol{b}, \nabla\phi \rangle d\boldsymbol{\mu}_n(t, i_n(w)) \right] dt \right| d\mathbb{P}(w) = 0 \tag{5.2}$$

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

Assume, besides conditions (a), (b), *and* (c) *above, that* (3.1) *has uniqueness in* $L_+^\infty([0, T]; L^1 \cap L^\infty(\mathbb{R}^d))$. *Then the* $\boldsymbol{\nu}$*-RLF* $\boldsymbol{\mu}(t, \mu)$ *relative to* $\boldsymbol{b}$ *exists, is unique, and*

$$\lim_{n\to\infty} \int_W \sup_{t\in[0,T]} d_{\mathscr{P}}\big(\boldsymbol{\mu}_n(t, i_n(w)), \boldsymbol{\mu}(t, i(w))\big) d\mathbb{P}(w) = 0. \tag{5.3}$$

PROOF. Let $(\boldsymbol{\eta}_n) \subset \mathscr{M}_+(\mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d)))$ be induced by $\boldsymbol{\mu}_n$ pushing forward $\boldsymbol{\nu}_n = (i_n)_\sharp\mathbb{P}$ via the map $\mu \mapsto (\mu, \boldsymbol{\mu}_n(t, \mu))$. Conditions (iii) and (iv) correspond, respectively, to conditions (i) and (ii) of Proposition 2.1; hence the marginals of $\boldsymbol{\eta}_n$ on $\Omega_T(\mathscr{P}(\mathbb{R}^d))$ are tight; since the first marginals, namely $\boldsymbol{\nu}_n$, are tight as well, a simple tightness criterion in product spaces (see, for instance, [7, lemma 5.2.2]) gives that $(\boldsymbol{\eta}_n)$ is tight. We consider a weak limit point $\boldsymbol{\eta}$ of

$(\boldsymbol{\eta}_n)$ and prove that $\boldsymbol{\eta}$ is the unique generalized $\boldsymbol{\nu}$-RLF relative to $\boldsymbol{b}$; this will give that the whole sequence $(\boldsymbol{\eta}_n)$ weakly converges to $\boldsymbol{\eta}$. Just to simplify notation, we assume that the whole sequence $(\boldsymbol{\eta}_n)$ weakly converges to $\boldsymbol{\eta}$.

We check conditions (i), (ii), and (iii) of Definition 3.9. First, since $\boldsymbol{\mu}_n(0,\mu) = \mu$ $\boldsymbol{\nu}_n$-a.e., we get $(e_0)_\sharp \boldsymbol{\eta}_n = \boldsymbol{\nu}_n$; hence $(e_0)_\sharp \boldsymbol{\eta} = \boldsymbol{\nu}$ and condition (i) is satisfied. Second, we check condition (iii): for $\phi \in C_c(\mathbb{R}^d)$ nonnegative, we have

$$\int_{\mathbb{R}^d} \phi \, d\mathbb{E}((e_t)_\sharp \boldsymbol{\eta}_n) = \int_{\mathbb{R}^d} \phi \, d\mathbb{E}(\boldsymbol{\mu}(t,\cdot)_\sharp \boldsymbol{\nu}_n) = \int_W \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w)) d\mathbb{P}(w),$$

and we can use assumption (i) to conclude that

$$\int_{\mathbb{R}^d} \phi \, d\mathbb{E}((e_t)_\sharp \boldsymbol{\eta}) \le C \int_{\mathbb{R}^d} \phi \, dz \quad \forall t \in [0,T], \tag{5.4}$$

so that condition (iii) is fulfilled.

Finally, we check condition (ii). Since $\boldsymbol{\eta}_n$ are concentrated on the closed set of pairs (μ,ω) with $\omega(0) = \mu$, the same is true for $\boldsymbol{\eta}$; it remains to show that $\omega(t)$ solves (1.24) for $\boldsymbol{\eta}$-a.e. (μ,ω). We shall denote by $\boldsymbol{\sigma} \in \mathscr{M}_+(\Omega_T(\mathscr{P}(\mathbb{R}^d)))$ the projection of $\boldsymbol{\eta}$ on the second factor and prove that (1.24) holds for $\boldsymbol{\sigma}$-a.e. ω.

We fix $\phi \in C_c^\infty(\mathbb{R}^d \setminus (S \times \mathbb{R}^n))$ and $\varphi \in C_c^\infty(0,T)$; we claim that the discontinuity set of the bounded map

$$\omega \mapsto \int_0^T \left[\varphi'(t) \int_{\mathbb{R}^d} \phi \, d\omega(t) + \varphi(t) \int_{\mathbb{R}^d} \langle \boldsymbol{b}, \nabla\phi \rangle d\omega(t)\right] dt \tag{5.5}$$

is $\boldsymbol{\sigma}$-negligible. Indeed, using (2.1) with $X = \mathbb{R}^d$ this discontinuity set is easily seen to be contained in

$$\left\{\omega \in \Omega_T(\mathscr{P}(\mathbb{R}^d)) : \int_0^T \omega(t)(\Sigma \times \mathbb{R}^n) dt > 0\right\}, \tag{5.6}$$

where Σ is the discontinuity set of $\boldsymbol{c}$. Since $\mathscr{L}^d(\Sigma \times \mathbb{R}^n) = 0$, by assumption (c), for all $t \in [0,T]$ inequality (5.4) gives $\omega(t)(\Sigma \times \mathbb{R}^n) = 0$ for $\boldsymbol{\sigma}$-a.e. ω; by Fubini's theorem in $[0,T] \times \Omega_T(\mathscr{P}(\mathbb{R}^d))$, we obtain that the set in (5.6) is $\boldsymbol{\sigma}$-negligible.

Now we write assumption (5.1) in terms of $\boldsymbol{\eta}_n$ as

$$\sup_{\delta>0} \limsup_{n\to\infty} \int_{\mathscr{P}(\mathbb{R}^d)\times\Omega_T(\mathscr{P}(\mathbb{R}^d))} \int_0^T \int_{B_R} \frac{1}{\operatorname{dist}^\beta(x,S)+\delta} \, d\omega(t)\, dt\, d\boldsymbol{\eta}_n(\mu,\omega) < \infty \qquad \forall R > 0,$$

and take the limit thanks to Fatou's lemma and the monotone convergence theorem to obtain

$$\int_{\Omega_T(\mathscr{P}(\mathbb{R}^d))} \int_0^T \int_{B_R} \frac{1}{\operatorname{dist}^\beta(x,S)} \, d\omega(t)\, dt\, d\boldsymbol{\sigma}(\omega) < \infty \quad \forall R > 0. \tag{5.7}$$

Next we write assumption (v) in terms of $\boldsymbol{\eta}_n$ as

$$\lim_{n\to\infty} \int_{\mathscr{P}(\mathbb{R}^d)\times\Omega_T(\mathscr{P}(\mathbb{R}^d))} \zeta \left| \int_0^T \left[\varphi'(t) \int_{\mathbb{R}^d} \phi \, d\omega(t) + \varphi(t) \int_{\mathbb{R}^d} \langle \boldsymbol{b}, \nabla\phi \rangle d\omega(t) \right] dt \right| d\boldsymbol{\eta}_n(\mu,\omega) = 0$$

with $\zeta \in C_b(\mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d)))$ nonnegative; then, the claim on the continuity of the map in (5.5) and (2.1) with $X = \mathscr{P}(\mathbb{R}^d) \times \Omega_T(\mathscr{P}(\mathbb{R}^d))$ allows us to conclude that

$$\int_{\mathscr{P}(\mathbb{R}^d)\times\Omega_T(\mathscr{P}(\mathbb{R}^d))} \zeta \left| \int_0^T \left[\varphi'(t) \int_{\mathbb{R}^d} \phi \, d\omega(t) + \varphi(t) \int_{\mathbb{R}^d} \langle \boldsymbol{b}, \nabla\phi \rangle d\omega(t) \right] dt \right| d\boldsymbol{\eta}(\mu,\omega) = 0.$$

Now we fix $\mathcal{A} \subset C_c^\infty(\mathbb{R}^d \setminus (S \times \mathbb{R}^n))$ and $\mathcal{B} \subset C_c^\infty(0,T)$ countable dense, and use the fact that ζ is arbitrary to find a $\boldsymbol{\sigma}$-negligible set $N \subset \Omega_T(\mathscr{P}(\mathbb{R}^d))$ such that

$$\int_0^T \left[\varphi'(t) \int_{\mathbb{R}^d} \phi \, d\omega(t) + \varphi(t) \int_{\mathbb{R}^d} \langle \boldsymbol{b}_t, \nabla\phi \rangle d\omega(t) \right] dt = 0 \quad \forall \phi \in \mathcal{A},\ \forall \varphi \in \mathcal{B},$$

for all $\omega \notin N$, and by a density argument we conclude that $\boldsymbol{\sigma}$ is concentrated on solutions to the continuity equation in $\mathbb{R}^d \setminus (S \times \mathbb{R}^n)$. By Lemma 5.1 and (5.7) we obtain that $\boldsymbol{\sigma}$-a.e. the continuity equation holds globally.

By Theorem 4.4 we know that the $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}(t,\mu)$ in $\mathscr{P}(\mathbb{R}^d)$ exists, is unique, and is related to the unique generalized $\boldsymbol{\nu}$-RLF $\boldsymbol{\eta}$ as in (3.3)–(3.4). This proves that we have convergence of the whole sequence $(\boldsymbol{\eta}_n)$ to $\boldsymbol{\eta}$. By applying Lemma 2.2 with $X = \mathscr{P}(\mathbb{R}^d)$ and $Y = \Omega_T(\mathscr{P}(\mathbb{R}^d))$, we conclude that (5.3) holds. □

In the next remark we consider some extensions of this result to the case when $\boldsymbol{b}$ satisfies (a) and (b) only, so that no information is available on the discontinuity set Σ of $\boldsymbol{c}$.

Remark 5.3. Assume that $\boldsymbol{b}$ satisfies (a) and (b) only. Then the conclusion of Theorem 5.2 is still valid, provided the asymptotic regularity condition (i) holds in a stronger form, namely,

$$\int_W \int_{\mathbb{R}^d} \phi \, d\boldsymbol{\mu}_n(t, i_n(w)) d\mathbb{P}(w) \le C \int_{\mathbb{R}^d} \phi \, dx \quad \forall \phi \in C_c(\mathbb{R}^d),\ \phi \ge 0,\ n \ge 1,$$

for some constant C independent of t. Indeed, assumption (c) was needed only to pass to the limit, in the weak convergence of $\boldsymbol{\eta}_n$ to $\boldsymbol{\eta}$, with test functions of the form (5.5). But if the stronger regularity condition above holds, convergence always holds by a density argument: first one checks this with $\boldsymbol{b}$ continuous and bounded on $\operatorname{supp}\phi$, and in this case the test function is continuous and bounded; then one approximates $\boldsymbol{b}$ in L^1 on $\operatorname{supp}\phi$ by bounded continuous functions.

6 Well-Posedness of the Continuity Equation with a Singular Potential

In this section we shall assume that $d = 2n$ and consider a more particular class of autonomous and Hamiltonian vector fields $\boldsymbol{b} : \mathbb{R}^d \to \mathbb{R}^d$ of the form

$$\boldsymbol{b}(z) = (p, -\nabla U(x)), \quad z = (x, p) \in \mathbb{R}^n \times \mathbb{R}^n.$$

Having in mind the application to the convergence of the Wigner-Husimi transforms in quantum molecular dynamics (see Section 7.2), we assume that:

(i) there exists a closed $\mathscr{L}^n$-negligible set $S \subset \mathbb{R}^n$ such that U is locally Lipschitz in $\mathbb{R}^n \setminus S$ and $\nabla U \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^n \setminus S; \mathbb{R}^n)$;

(ii) $U(x) \to +\infty$ as $x \to S$;

(iii) U satisfies

$$\operatorname*{ess\,sup}_{U(x)\le M} \frac{|\nabla U(x)|}{1+|x|} < \infty \quad \forall M \ge 0. \tag{6.1}$$

THEOREM 6.1 *Under assumptions* (i), (ii), (iii), *the continuity equation* (3.1) *has existence and uniqueness in* $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$.

PROOF. *Uniqueness*. Let $w_t \in L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$ be a solution to (3.1), and consider a smooth compactly supported function $\phi : \mathbb{R} \to \mathbb{R}^+$. Set $E = E(x,p) := \frac{1}{2}|p|^2 + U(x)$. Then, since U is locally Lipschitz on sublevels $\{U \le \ell\}$ for any $\ell \in \mathbb{R}$ (by (i) and (ii)), $\phi \circ E$ is uniformly bounded and locally Lipschitz in $\mathbb{R}^d$. Moreover,

$$\langle \nabla(\phi \circ E)(z), \boldsymbol{b}(z)\rangle = \phi'(E(z))\langle \nabla E(z), \boldsymbol{b}(z)\rangle = 0 \quad \text{for } \mathscr{L}^d\text{-a.e. } z \in \mathbb{R}^d,$$

and we easily deduce that $(\phi \circ E)w_t \in L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$ also solves equation (3.1).

Let $M > 0$ be large enough so that $\operatorname{supp}\phi \subset [-M, M]$, and let $\psi : \mathbb{R} \to \mathbb{R}^+$ be a smooth cutoff function such that $\psi \equiv 1$ on $[-M, M]$. Then $\phi \circ E = (\psi \circ E)(\phi \circ E)$, which implies that $(\phi \circ E)w_t$ solves (3.1) with the vector field $\widetilde{\boldsymbol{b}} := (\psi \circ E)\boldsymbol{b}$. Now, thanks to (i) through (iii), it is easily seen that the following properties hold:

$$\widetilde{\boldsymbol{b}} \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^d; \mathbb{R}^d), \quad \operatorname*{ess\,sup} \frac{|\widetilde{\boldsymbol{b}}|(z)}{1+|z|} < \infty. \tag{6.2}$$

Indeed, the first one is a direct consequence of (i) and (ii), while the second one follows from (ii) and (iii) and the simple estimate

$$\operatorname*{ess\,sup}_{E(z)\le M'} \frac{|\boldsymbol{b}(z)|}{1+|z|} \le \left(\sup \frac{|p|}{1+|p|}\right) + \left(\operatorname*{ess\,sup}_{U(x)\le M'} \frac{|\nabla U(x)|}{1+|x|}\right) < \infty \quad \forall M' > 0.$$

Thanks to (6.2), we can apply [2, theorems 34 and 26] to deduce that $(\phi \circ E)w_t$ is unique, given the initial condition $\mu_0 = (\phi \circ E)w_0\mathscr{L}^d$. Since $E(z)$ is finite for $\mathscr{L}^d$-a.e. z, by the arbitrariness of ϕ we easily obtain that w_t is unique, given the initial condition w_0.

Existence. We now want to prove existence of solutions in $L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$. Let $\bar{w} \in L^1 \cap L^\infty(\mathbb{R}^d)$ be nonnegative and let us consider a sequence of smooth globally Lipschitz functions V_k with $|\nabla V_k - \nabla U| \to 0$ in $L^1_{\text{loc}}(\mathbb{R}^n)$; standard results imply the existence of nonnegative solutions w^k to the continuity equation with velocity $\boldsymbol{b}^k := (p, -\nabla V_k)$ with $w^k_0 = \bar{w}$, $\int_{\mathbb{R}^d} w^k_t \, dx \, dp = \int_{\mathbb{R}^d} w^k_0 \, dx \, dp$ and with $\|w^k_t\|_\infty \le \|w^k_0\|_\infty$ (they are the pushforward of w^k_0 under the flow map of $\boldsymbol{b}^k$). Since $\phi \mapsto \int_{\mathbb{R}^d} w^k_t \phi \, dx \, dp$ are equicontinuous for all $\phi \in C^1_c(\mathbb{R}^d)$, we can assume the existence of $w \in L^\infty_+([0,T]; L^1 \cap L^\infty(\mathbb{R}^d))$ with $w^k_t \to w_t$ weakly, in the duality with $C^1_c(\mathbb{R}^d)$, for all $t \ge 0$. Taking the limit as $k \to \infty$ immediately gives that w_t is a solution to (3.1). □

THEOREM 6.2 *The ν-RLF $(\boldsymbol{x}(t,x,p), \boldsymbol{p}(t,x,p))$ in $\mathbb{R}^{2n}$ and the $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}(t,\mu)$ in $\mathscr{P}(\mathbb{R}^{2n})$ relative to $\boldsymbol{b}(x,p) := (p, -\nabla U(x))$ exist and are unique under assumptions* (i), (ii), *and* (iii). *They are related by*

$$\boldsymbol{\mu}(t,\mu) = \int_{\mathbb{R}^{2d}} \delta_{(\boldsymbol{x}(t,x,p),\boldsymbol{p}(t,x,p))} d\mu(x,p). \tag{6.3}$$

PROOF. Existence and uniqueness of the ν-RLF in $\mathbb{R}^d$ follow by Theorems 6.1 and 4.1. The existence of the ν-RLF implies the existence of the $\boldsymbol{\nu}$-RLF $\boldsymbol{\mu}$ in (6.3) by Theorem 4.2, and the well-posedness of the continuity equation with velocity $\boldsymbol{b}$, together with the existence of the generalized $\boldsymbol{\nu}$-RLF induced by $\boldsymbol{\mu}$ (see (3.3) and (3.4)), yield the uniqueness of $\boldsymbol{\mu}$ by Theorem 4.4. □

7 Estimates on Solutions to (1.1) and on Error Terms

In this section we collect some a priori estimates on solutions to (1.1) and on the error terms $\mathscr{E}_\varepsilon(U,\psi)$ and $\mathscr{E}'_\varepsilon(U,\psi)$, appearing in (1.13) and (1.16), respectively.

We recall that the Husimi transform $\psi \mapsto \widetilde{W}_\varepsilon\psi$ can be defined in terms of convolution of the Wigner transform with the $2n$-dimensional Gaussian kernel with variance $\varepsilon/2$:

$$G^{(2n)}_\varepsilon(x,p) := \frac{e^{-(|x|^2+|p|^2)/\varepsilon}}{(\pi\varepsilon)^n} = G^{(n)}_\varepsilon(x) G^{(n)}_\varepsilon(p), \tag{7.1}$$

namely, $\widetilde{W}_\varepsilon\psi = (W_\varepsilon\psi) * G^{(2n)}_\varepsilon$. It turns out that the asymptotic behavior as $\varepsilon \to 0$ is the same for the Wigner and the Husimi transform (see also (7.7) below for a more precise statement).

For later use, we recall that the x-marginal of $W_\varepsilon\psi$ is the position density $|\psi|^2\mathscr{L}^n$. Also, the change of variables

$$\begin{cases} x + \frac{\varepsilon}{2}\, y = u \\ x - \frac{\varepsilon}{2}\, y = u' \end{cases} \tag{7.2}$$

and a simple computation show that the p-marginal of $W_\varepsilon\psi$ is the momentum density, namely $(2\pi\varepsilon)^{-n}|\mathcal{F}\psi|^2(p/\varepsilon)\mathscr{L}^n$. (Strictly speaking, these identities are only true in the sense of principal values, since $W_\varepsilon\psi$, despite tending to 0 as $|(x,p)| \to \infty$, does not in general belong to L^1.) Since the Gaussian kernel $G_\varepsilon^{(2n)}(x,p)$ in (7.1) has a product structure, it turns out that

$$\int_{\mathbb{R}^n} \widetilde{W}_\varepsilon\psi(x,p)dp = \int_{\mathbb{R}^n} |\psi|^2(x-x')G_\varepsilon^{(n)}(x')dx', \tag{7.3}$$

$$\int_{\mathbb{R}^n} \widetilde{W}_\varepsilon\psi(x,p)dx = \left(\frac{1}{2\pi\varepsilon}\right)^n \int_{\mathbb{R}^n} |\mathcal{F}\psi|^2\left(\frac{p-p'}{\varepsilon}\right)G_\varepsilon^{(n)}(p')dp'. \tag{7.4}$$

Since $\widetilde{W}_\varepsilon\psi$ is nonnegative (see Section 8 for details), the two identities above hold in the standard sense.

As in [24] we shall consider the completion $\mathcal{A}$ of $C_c^\infty(\mathbb{R}^{2n})$ with respect to the norm

$$\|\varphi\|_{\mathcal{A}} := \int_{\mathbb{R}^n} \sup_{x\in\mathbb{R}^n} |\mathcal{F}_p\varphi|(x,y)dy, \quad \varphi \in C_c^\infty(\mathbb{R}^{2n}), \tag{7.5}$$

where $\mathcal{F}_p$ denotes the partial Fourier transform with respect to p, that is,

$$\mathcal{F}_p\varphi(x,y) = \int_{\mathbb{R}^n} e^{-ip\cdot y}\varphi(x,p)dp.$$

It is easily seen that $\sup|\varphi| \le \|\varphi\|_{\mathcal{A}}$; hence $\mathcal{A}$ is contained in $C_b(\mathbb{R}^{2n})$ and $\mathscr{M}(\mathbb{R}^{2n})$ canonically embeds into $\mathcal{A}'$ (the embedding is injective by the density of $C_c^\infty(\mathbb{R}^{2n})$). The norm of $\mathcal{A}$ is technically convenient because of the simple estimate

$$\left|\int_{\mathbb{R}^{2n}} \varphi W_\varepsilon\psi\, dx\, dp\right| \le \frac{1}{(2\pi)^n}\|\varphi\|_{\mathcal{A}}\,\|\psi\|_2^2. \tag{7.6}$$

Since for all $\varphi \in C_c^\infty(\mathbb{R}^{2n})$ one has $\varphi * G_\varepsilon^{(2n)} \to \varphi$ in $\mathcal{A}$ as $\varepsilon \downarrow 0$, it follows that

$$\lim_{\varepsilon\downarrow 0}\left[\int_{\mathbb{R}^d} \varphi W_\varepsilon\psi\, dx\, dp - \int_{\mathbb{R}^d} \varphi \widetilde{W}_\varepsilon\psi\, dx\, dp\right] = 0 \tag{7.7}$$

uniformly on bounded subsets of $L^2(\mathbb{R}^d;\mathbb{C})$. This will obviously be an ingredient in transferring the dynamical properties from the Wigner to the Husimi transforms.

If $\{\varphi_k\}_{k\geq 1} \subset C_c^\infty(\mathbb{R}^{2n})$ is a dense set in the unit ball of $\mathcal{A}$, we shall also consider the explicit distance

$$d_{\mathcal{A}'}(L_1, L_2) := \sum_{k=1}^{\infty} \min\{|\langle L_1 - L_2, \varphi_k\rangle|, 2^{-k}\} \tag{7.8}$$

inducing the weak-$*$ topology in norm bounded subsets of $\mathcal{A}'$.

7.1 The PDE Satisfied by the Husimi Transforms

In this short section we see how (1.13) is modified in passing from the Wigner to the Husimi transform. Denoting by $\tau_{(y,q)}$ the translation in phase space induced by $(y,q) \in \mathbb{R}^n \times \mathbb{R}^n$, we obtain from (1.13)

$$\partial_t \tau_{(y,q)} W_\varepsilon \psi_t^\varepsilon + (p-q)\cdot \nabla_x \tau_{(y,q)} W_\varepsilon \psi_t^\varepsilon = \tau_{(y,q)} \mathscr{E}_\varepsilon(U, \psi_t^\varepsilon)$$

in the sense of distributions. Since $\widetilde{W}_\varepsilon \psi_t^\varepsilon$ is an average of translates of $W_\varepsilon \psi_t^\varepsilon$, we get (still in the sense of distributions)

$$\partial_t \widetilde{W}_\varepsilon \psi_t^\varepsilon + p \cdot \nabla_x \widetilde{W}_\varepsilon \psi_t^\varepsilon = \mathscr{E}_\varepsilon(U, \psi_t^\varepsilon) * G_\varepsilon^{(2n)} + \sqrt{\varepsilon}\nabla_x \cdot \left[W_\varepsilon \psi_t^\varepsilon * \bar{G}_\varepsilon^{(2n)}\right], \tag{7.9}$$

where

$$\bar{G}_\varepsilon^{(2n)}(y,q) := \frac{q}{\sqrt{\varepsilon}} G_\varepsilon^{(2n)}(y,q). \tag{7.10}$$

Indeed, we have

$$-\int_{\mathbb{R}^{2n}} q \cdot \nabla_x \tau_{(y,q)} W_\varepsilon \psi_t^\varepsilon G_\varepsilon^{(2n)}(y,q)\,dy\,dq = -\sqrt{\varepsilon}\nabla_x \cdot [W_\varepsilon \psi_t^\varepsilon * \bar{G}_\varepsilon^{(2n)}].$$

Although we will not use it here, let us mention that it is possible to derive a closed equation (i.e., one not involving $W_\varepsilon \psi_t^\varepsilon$) for $\widetilde{W}_\varepsilon \psi_t^\varepsilon$ (see [8, 9, 10] for applications to the semiclassical limit in strong topology).

7.2 Assumptions on U and Regularity of Born-Oppenheimer Potentials

We assume that $n = 3M$, $x = (x_1, \dots, x_M) \in (\mathbb{R}^3)^M$, and $U = U_s + U_b$, with

(A) U_s the (repulsive) Coulomb potential (1.7),

(B) U_b globally bounded and Lipschitz, with $\nabla U_b \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^n \setminus S; \mathbb{R}^n)$,

where S, the singular set of Section 5 and Section 6, is given by

$$S = \bigcup_{1\leq \alpha<\beta\leq M} S_{\alpha\beta} \quad \text{with } S_{\alpha\beta} := \{x \in \mathbb{R}^n : x_\alpha = x_\beta\}.$$

We claim that assumptions (A) and (B) are exactly satisfied when U is a Born-Oppenheimer molecular potential energy surface (1.7), (1.8), and (1.9). Boundedness and Lipschitz continuity of U_b follow from standard estimates, and the finer property $\nabla U_b \in \mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^n \setminus S; \mathbb{R}^n)$ was observed in [19]. Since that latter work has not yet appeared (and even for boundedness and Lipschitz continuity of U_b, which is certainly well-known, we know of no other reference than [19]), we include a full derivation of these properties in the case of two atoms.

PROPOSITION 7.1 *Let U_b be the Born-Oppenheimer potential energy* (1.8)–(1.9). *Then U_b is globally bounded and Lipschitz and, if $M = 2$ (diatomic case), $\nabla U_b \in$* $\mathrm{BV}_{\mathrm{loc}}(\mathbb{R}^n \setminus S; \mathbb{R}^n)$.

PROOF. By the Rayleigh-Ritz variational principle,

$$U_b(x) := \inf\{E[1, v_x, w, \Psi] \mid \Psi \in \mathcal{A}_N\}, \tag{7.11}$$

where N stands for the number of electrons and

$$\begin{aligned} E[\gamma, v_x, w, \Psi] &= T[\gamma, \Psi] + V_{ne}[v_x, \Psi] + V_{ee}[w, \Psi], \\ T[\gamma, \Psi] &= \frac{\gamma}{2} \int_{(\mathbb{R}^3\times\mathbb{Z}_2)^N} |\nabla\Psi|^2, \\ V_{ne}[v_x, \Psi] &= \int_{(\mathbb{R}^3\times\mathbb{Z}_2)^N} \sum_{i=1}^{N} v_x(r_i)|\Psi|^2, \\ V_{ee}[w, \Psi] &= \int_{(\mathbb{R}^3\times\mathbb{Z}_2)^N} \sum_{1\le i<j\le N} w(r_i - r_j)|\Psi|^2. \end{aligned} \tag{7.12}$$

Here $v_x = -\sum_{\alpha=1}^{M} Z_\alpha|\cdot - x_\alpha|^{-1}$, $w = |\cdot|^{-1}$, and the set of admissible trial functions is given by $\mathcal{A}_N = \{\Psi \in H^1((\mathbb{R}^3 \times \mathbb{Z}_2)^N) \mid \|\Psi\|_2 = 1,\ \Psi \text{ antisymmetric}\}$, where antisymmetric means that, with space-spin coordinates $z_i = (r_i, s_i) \in \mathbb{R}^3 \times \mathbb{Z}_2$, $\Psi(\dots, z_i, \dots, z_j, \dots) = -\Psi(\dots, z_j, \dots, z_i, \dots)$ for all $i \neq j$. Note that the coordinates $x = (x_1, \dots, x_M) \in \mathbb{R}^{3M}$ of the nuclei on which U_b depends enter only through the location of the Coulomb singularities in the potential v_x.

Uniform boundedness of U_b follows by appropriate Hölder and Sobolev estimates, e.g., the estimates [18, eqs. (1.3), (1.4)]:

$$\begin{aligned} |V_{ne}[v_x, \Psi]| &\le c_S \|v_x^{(1)}\|_{3/2}\, \|\nabla\Psi\|_2^2 + N\|v_x^{(2)}\|_\infty\, \|\Psi\|_2^2, \\ |V_{ee}[w, \Psi]| &\le c_S \frac{N-1}{2} \|w^{(1)}\|_{3/2}\, \|\nabla\Psi\|_2^2 + \binom{N}{2} \|w^{(2)}\|_\infty\, \|\Psi\|_2^2. \end{aligned}$$

Here c_S is the Sobolev constant in the inequality $\|u\|_6^2 \le c_S\|\nabla u\|_2^2$ in $\mathbb{R}^3$, and the potentials v_x and w have been decomposed into $v_x = v_x^{(1)} + v_x^{(2)}$ and $w = w^{(1)} + w^{(2)}$ with $v_x^{(1)}, w^{(1)} \in L^{3/2}(\mathbb{R}^3)$ and $v_x^{(2)}, w^{(2)} \in L^\infty(\mathbb{R}^3)$. (Note the well-known fact that it is important that one uses Sobolev estimates in $\mathbb{R}^3$, not $\mathbb{R}^{3N}$, as the latter would only give $|\Psi|^2 \in L^{N/(N-2)}$, but $v_x(r_i)$ does not locally belong to the corresponding dual L^p space.) One now observes that the above decomposition can be chosen in such a way that the $L^{3/2}$-norms of $v_x^{(1)}$ and $w^{(1)}$ are small independently of x, and the L^∞-norms of $v_x^{(2)}$ and $w^{(2)}$ are bounded independently of x. Hence, taking advantage of the positive contribution coming from $T[1,\Psi]$, we see that U_b is globally bounded from below.

To see that U_b is globally Lipschitz, note first that from the above arguments we know that the infimum in (7.11) can be restricted to functions in $\mathcal{A}_N$ satisfying the bound $\|\nabla\Psi\|_2 \le C$ for some uniform constant C independent of x. Now for each such fixed Ψ we can write

$$|E[\gamma, v_{x+h}, w, \Psi] - E[\gamma, v_x, w, \Psi]| = |V_{ne}[v_{x+h} - v_x, \Psi]|. \tag{7.13}$$

We now estimate

$$\begin{aligned} |v_{x+h}(r_i) - v_x(r_i)| &= \left| \int_0^1 \frac{d}{dt} v_{x+th}(r_i)dt \right| \\ &\le \sum_{\alpha=1}^{M} Z_\alpha |h_\alpha| \int_0^1 \frac{1}{|r_i - (x_\alpha + th_\alpha)|^2}\, dt \end{aligned}$$

and apply Hardy's inequality in $\mathbb{R}^3_{r_i}$,

$$\int\limits_{\mathbb{R}^3} \frac{|u(r_i)|^2}{|r_i - a|^2}\, dr_i \le 4 \int\limits_{\mathbb{R}^3} |\nabla u(r_i)|^2\, dr_i .$$

It follows that the right-hand side of (7.13) is bounded from above by

$$\sum_{\alpha=1}^{M} Z_\alpha |h_\alpha| \cdot 4 \|\nabla\Psi\|_2^2 .$$

This shows that U_b can be written as the infimum of uniformly Lipschitz functions, completing the proof of global Lipschitz continuity.

Finally, we come to the proof of the asserted BV regularity of U_b in the case $M = 2$. The key to understanding this lies in the simple but important observation that the energy functional E in (7.12) is affine in each of γ, v_x, and w, and hence U_b, being an infimum over affine functions, is concave in each of γ, v_x, and w. It remains to convert concavity in the potential v_x into BV regularity *of* U_b. A particularly short argument can be given for diatomic molecules: Let $R := |x_1 - x_2|$. By translation invariance and frame indifference of U_b, i.e., $U_b(x_1, x_2) = U_b(Ox_1 + a, Ox_2 + a)$ for any $O \in \mathrm{SO}(3)$ and any $a \in \mathbb{R}^3$, U_b is only a function of $R := |x_1 - x_2|$. So we may without loss of generality assume $x_1 = 0$, $x_2 = Re_1$, where $e_1 = (1, 0, 0)$. We now exploit the scaling of the different energy contributions with respect to simultaneous dilation by a factor $\zeta > 0$ of the positions of nuclei and electrons, $x \mapsto \zeta^{-1}x$, $\Psi \mapsto \Psi_\zeta(r_1, s_1, \ldots, r_N, s_N) = \zeta^{3N/2}\Psi(\zeta r_1, s_1, \ldots, \zeta r_N, s_N)$:

$$\begin{gathered} T[\gamma, \Psi_\zeta] = T[\zeta^2\gamma, \Psi], \quad V_{ne}[v_{\zeta^{-1}x}, \Psi_z] = \zeta V_{ne}[v_x, \Psi], \\ V_{ee}[w, \Psi_\zeta] = \zeta V_{ee}[w, \Psi]. \end{gathered}$$

It follows that $E[\gamma, v_x, w, \Psi] = \zeta^{-1} E[\zeta^{-1}\gamma, v_{\zeta^{-1}x}, w, \Psi_\zeta]$. Note that the map $\Psi \mapsto \Psi_\zeta$ preserves the L^2-norm and is a bijection of $\mathcal{A}_N$.

Taking the infimum over Ψ and setting $\zeta := R$ yields

$$U_b((0, Re_1)) = \frac{1}{R^2}\phi(R) \tag{7.14}$$

with $\phi(R) := \inf\{E[1, Rv_{(0,e_1)}, Rw, \Psi] \mid \Psi \in \mathcal{A}_N\}$. Now ϕ, being the infimum of affine functions, is a concave function, and hence its derivative ϕ' belongs to the space $\mathrm{BV}_{\mathrm{loc}}((0,\infty))$. Altogether we have shown that

$$U_b(x_1, x_2) = |x_1 - x_2|^{-2}\phi(|x_1 - x_2|) \quad \text{with } \phi' \in \mathrm{BV}_{\mathrm{loc}}((0,\infty)).$$

Standard arguments then imply that ∇U_b is locally BV in the complement of S, S being the singular set $\{x_1 = x_2\}$. The proof of the proposition is complete. □

We note that assumptions (A) and (B) on U_s and U_b immediately imply

$$U_s(x) \geq \frac{c}{\operatorname{dist}(x, S)} \tag{7.15}$$

with $c > 0$ depending only on the numbers Z_α in (1.7).

The vector field $\boldsymbol{b} = (p, -\nabla U)$ satisfies assumptions (a) and (b) of Section 5 and assumptions (i) through (iii) of Section 6, so that the ν-RLF in $\mathbb{R}^{2n}$ and the $\boldsymbol{\nu}$-RLF in $\mathscr{P}(\mathbb{R}^{2n})$ relative to $\boldsymbol{b}$ exist and are unique, and the stability result of Section 5 can be applied, as we will show in Section 9.

7.3 Estimates on Solutions to (1.1)

Towards our goal of verifying assumptions (i) through (v) of Theorem 5.2, we will need the following properties of the solutions to (1.1), which are obtained by standard results on the unitary propagator e^{-itH_ε} or are shown in detail in [6].

CONSERVED QUANTITIES

$$\int_{\mathbb{R}^n} \frac{1}{2}|\varepsilon\nabla\psi_t^\varepsilon|^2 + U|\psi_t^\varepsilon|^2\,dx = \int_{\mathbb{R}^n} \frac{1}{2}|\varepsilon\nabla\psi_0^\varepsilon|^2 + U|\psi_0^\varepsilon|^2\,dx \quad \forall t \in \mathbb{R}, \tag{7.16}$$

$$\int_{\mathbb{R}^n} |H_\varepsilon\psi_t^\varepsilon|^2\,dx = \int_{\mathbb{R}^n} |H_\varepsilon\psi_0^\varepsilon|^2\,dx \quad \forall t \in \mathbb{R}. \tag{7.17}$$

A PRIORI ESTIMATE [6, lemma 5.1]

$$\sup_{t\in\mathbb{R}} \int_{\mathbb{R}^n} U_s^2|\psi_t^\varepsilon|^2\,dx \leq \int_{\mathbb{R}^n} |H_\varepsilon\psi_0^\varepsilon|^2\,dx + 2\sup|U_b|\bigg(\int_{\mathbb{R}^n} \langle\psi_0^\varepsilon, H_\varepsilon\psi_0^\varepsilon\rangle dx + \sup|U_b|\bigg). \tag{7.18}$$

TIGHTNESS IN SPACE [6, lemma 3.3]

$$\sup_{t\in[-T,T]} \int\limits_{\mathbb{R}^n\setminus B_{2R}} |\psi_t^\varepsilon|^2\, dx \le \int\limits_{\mathbb{R}^n\setminus B_R} |\psi_0^\varepsilon|^2(x)dx + cT\frac{1+\int\langle\psi_0^\varepsilon, H_\varepsilon\psi_0^\varepsilon\rangle dx}{R} \tag{7.19}$$

with c depending only on n.

7.4 Estimates and Convergence of $\mathscr{E}_\varepsilon(U_b,\psi)$

In this section we prove some estimates for and the convergence of the term $\mathscr{E}_\varepsilon(U_b,\psi)$, as defined in (1.14). In particular, we use averaging with respect to the "random" parameter w to derive new estimates on $\mathscr{E}_\varepsilon(V,\psi_w^\varepsilon)$, with V Lipschitz only, so that the estimates are applicable to $V = U_b$.

The first basic estimate on $\mathscr{E}_\varepsilon(V,\psi)$, for ψ with unit L^2-norm, can be obtained, when V is Lipschitz, by estimating the difference quotient in the square brackets in (1.14) with the Lipschitz constant:

$$\left|\int\limits_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V,\psi)\phi\, dx\, dp\right| \le \frac{1}{(2\pi)^n}\|\nabla V\|_\infty \int\limits_{\mathbb{R}^n} |y| \sup_{x\in\mathbb{R}^n} |\mathcal{F}_p\phi|(x,y)dy. \tag{7.20}$$

In order to derive a more refined estimate, we consider families ψ_w^ε indexed by a parameter $w\in W$, with $(W,\mathcal{F},\mathbb{P})$ a probability space, satisfying

$$\sup_{\varepsilon>0}\ \sup_{(x,p)\in\mathbb{R}^{2n}} \int\limits_W \widetilde{W}_\varepsilon\psi_w^\varepsilon(x,p)d\mathbb{P}(w) < \infty, \tag{7.21}$$

$$\sup_{\varepsilon>0}\ \sup_{x\in\mathbb{R}^n} \int\limits_W |\psi_w^\varepsilon * G_{\lambda\varepsilon^2}^{(n)}|^2(x)d\mathbb{P}(w) \le C(\lambda) < \infty \quad \forall\lambda>0. \tag{7.22}$$

Under these assumptions, our first convergence result reads as follows:

THEOREM 7.2 (Convergence of Error Term I) *Let $\psi_w^\varepsilon\in L^2(\mathbb{R}^n;\mathbb{C})$ be normalized wave functions satisfying* (7.21) *and* (7.22)*, and let $V:\mathbb{R}^n\to\mathbb{R}$ be Lipschitz. Then*

$$\lim_{\varepsilon\to 0}\int\limits_W\left|\int\limits_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V,\psi_w^\varepsilon)\phi\, dx\, dp + \int\limits_{\mathbb{R}^{2n}} \langle\nabla V,\nabla_p\phi\rangle\widetilde{W}_\varepsilon\psi_w^\varepsilon dx\, dp\right| d\mathbb{P}(w) = 0 \quad \forall\phi\in C_c^\infty(\mathbb{R}^{2n}). \tag{7.23}$$

PROOF. The proof is achieved by a density argument. The first remark is that linear combinations of tensor functions $\phi(x,p) = \phi_1(x)\phi_2(p)$, $\phi_i\in C_c^\infty(\mathbb{R}^n)$, are dense for the norm considered in (7.20). 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 V is of class C^2 (by the arguments in [6, 24]; see also the splitting argument in the y-space in the proof of Theorem 7.4). Hence combining the two remarks and using the linearity of the error term with respect to the potential V, we can prove convergence by a density argument, by approximating V uniformly and in $W^{1,2}$ topology on the support of ϕ_1 by potentials $V_k \in C^2(\mathbb{R}^n)$ with uniformly Lipschitz constants; then, setting $A_k = (V - V_k)\phi_1$ and choosing a sequence λ_k in Proposition 7.3 converging slowly to 0 in such a way that $\|\nabla A_k\|_2 \to 0$ much faster than $1/\sqrt{C(\lambda_k)}$, we obtain

$$\lim_{k\to\infty} \sup_{\varepsilon>0} \int_W \left| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V - V_k, \psi_w^\varepsilon)(x,p)\phi_1(x)\phi_2(p)\,dx\,dp \right| d\mathbb{P}(w) = 0.$$

As for the term in (7.23) involving the Wigner transforms, we can use (7.21) to obtain that

$$\limsup_{k\to\infty} \sup_{\varepsilon>0} \int_W \left| \int_{\mathbb{R}^{2n}} \widetilde{W}_\varepsilon \psi_w^\varepsilon \langle \nabla(V - V_k), \nabla\phi_2\rangle \phi_1\,dx\,dp \right| d\mathbb{P}(w)$$

can be estimated from above with a constant multiple of

$$\limsup_{k\to\infty} \int_{\mathbb{R}^n} |\phi_1|\,|\nabla V - \nabla V_k|\,dx \int_{\mathbb{R}^n} |\nabla\phi_2|(p)\,dp = 0.$$

□

We shall actually use the conclusion of Theorem 7.2 in the form

$$\lim_{\varepsilon\to0} \int_W \left| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V, \psi_w^\varepsilon)\phi * G_\varepsilon^{(2n)}\,dx\,dp + \int_{\mathbb{R}^{2n}} \langle \nabla V, \nabla_p \phi\rangle \widetilde{W}_\varepsilon \psi_w^\varepsilon\,dx\,dp \right| d\mathbb{P}(w) = 0 \quad \forall \phi \in C_c^\infty(\mathbb{R}^{2n}) \tag{7.24}$$

with ϕ replaced by $\phi * G_\varepsilon^{(2n)}$ in the first summand, in the factor of $\mathscr{E}_\varepsilon(V, \psi_w^\varepsilon)$; this formulation is equivalent thanks to (7.20).

PROPOSITION 7.3 (A Priori Estimate) *Let $\psi_w^\varepsilon \in L^2(\mathbb{R}^n;\mathbb{C})$ be unitary wave functions satisfying* (7.22) *and let $\phi_1, \phi_2 \in C_c^\infty(\mathbb{R}^n)$. Then, for all $V : \mathbb{R}^n \to \mathbb{R}$ Lipschitz and all $\lambda > 0$, we have that*

$$\int_W \left| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V, \psi_w^\varepsilon)(x,p)\phi_1(x)\phi_2(p)\,dx\,dp \right| d\mathbb{P}(w) \tag{7.25}$$

can be estimated from above by

$$\begin{aligned}
&\|\phi_1\|_\infty \|\nabla V\|_\infty \int_{\mathbb{R}^n} |y||\mathcal{F}_p\phi_2(y) - \mathcal{F}_p\phi_2 * G_\lambda^{(n)}(y)|dy \\
&\quad + \sqrt{\lambda}\|\nabla A\|_\infty \|\mathcal{F}_p\phi_2\|_1 \int_{\mathbb{R}^n} |u|G_1^{(n)}(u)du \\
&\quad + \sqrt{C(\lambda)}\|\nabla A\|_2 \int_{\mathbb{R}^n} |z|\,|\mathcal{F}_p\phi_2|(z)dz \\
&\quad + \|V\|_\infty \|\nabla\phi_1\|_\infty \int_{\mathbb{R}^n} |y|\,\big|\mathcal{F}_p\phi_2 * G_\lambda^{(n)}\big|(y)dy.
\end{aligned} \tag{7.26}$$

where $A := V\phi_1$ and $C(\lambda)$ is given in (7.22).

PROOF. Set $\widehat{\phi}_2 = \mathcal{F}_p\phi_2$; since (7.20) gives that

$$\left|\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V,\psi_w^\varepsilon)\phi_1(x)\phi_2(p)dx\,dp - \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(V,\psi_w^\varepsilon)\phi_1(x)\phi_2(p)e^{-|p|^2\lambda/4}\,dx\,dp\right|$$

can be estimated from above with $\|\phi_1\|_\infty \|\nabla V\|_\infty \int |y|\,|\widehat{\phi}_2(y) - \widehat{\phi}_2 * G_\lambda^{(n)}(y)|dy$, we recognize the first error term in (7.26), and we will estimate the integral of $\mathscr{E}_\varepsilon(V,\psi_w^\varepsilon)$ against $\phi_1(x)\phi_2(p)e^{-|p|^2\lambda/4}$, namely,

$$\int_W\int_{\mathbb{R}^{2n}} \frac{V(x+\frac{\varepsilon}{2}y) - V(x-\frac{\varepsilon}{2}y)}{\varepsilon}\phi_1(x)\widehat{\phi}_2 * G_\lambda^{(n)}(y) \psi_w^\varepsilon\Big(x+\frac{\varepsilon}{2}y\Big)\overline{\psi_w^\varepsilon\Big(x-\frac{\varepsilon}{2}y\Big)}dx\,dy\,d\mathbb{P}(w).$$

In addition, we split this expression as the sum of three terms, namely

$$\mathrm{I} := \int_W\int_{\mathbb{R}^{2n}} \frac{A(x+\frac{\varepsilon}{2}y) - A(x-\frac{\varepsilon}{2}y)}{\varepsilon}\widehat{\phi}_2 * G_\lambda^{(n)}(y) \psi_w^\varepsilon\Big(x+\frac{\varepsilon}{2}y\Big)\overline{\psi_w^\varepsilon\Big(x-\frac{\varepsilon}{2}y\Big)}dx\,dy\,d\mathbb{P}(w), \tag{7.27}$$

$$\mathrm{II} := \int_W\int_{\mathbb{R}^{2n}} V\Big(x+\frac{\varepsilon}{2}y\Big)\frac{\phi_1(x) - \phi_1(x+\frac{\varepsilon}{2}y)}{\varepsilon}\widehat{\phi}_2 * G_\lambda^{(n)}(y) \psi_w^\varepsilon\Big(x+\frac{\varepsilon}{2}y\Big)\overline{\psi_w^\varepsilon\Big(x-\frac{\varepsilon}{2}y\Big)}dx\,dy\,d\mathbb{P}(w), \tag{7.28}$$

$$\text{(7.29)}\quad \mathrm{III} := -\int_W \int_{\mathbb{R}^{2n}} V\left(x - \frac{\varepsilon}{2}y\right) \frac{\phi_1(x) - \phi_1(x - \frac{\varepsilon}{2}y)}{\varepsilon} \widehat{\phi}_2 * G_\lambda^{(n)}(y) \psi_w^\varepsilon\left(x + \frac{\varepsilon}{2}y\right) \overline{\psi_w^\varepsilon\left(x - \frac{\varepsilon}{2}y\right)} dx\,dy\,d\mathbb{P}(w).$$

The most difficult term to estimate is (7.27), since both (7.28) and (7.29) can be easily estimated from above with $\frac{1}{2}\|V\|_\infty \|\nabla\phi_1\|_\infty \int_{\mathbb{R}^n} |y|\,|\widehat{\phi}_2 * G_\lambda^{(n)}|(y)dy$. We first perform some manipulations of this expression, omitting for simplicity the integration with respect to w; then we will estimate the resulting terms taking (7.22) into account.

We expand the convolution product and make the change of variables (7.2) to get

$$\text{(7.30)}\quad \frac{1}{(\pi\lambda)^{n/2}\varepsilon^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^{2n}} \frac{A(u) - A(u')}{\varepsilon} e^{-\frac{|\varepsilon z - (u-u')|^2}{\varepsilon^2\lambda}} \psi_w^\varepsilon(u) \overline{\psi_w^\varepsilon(u')} \widehat{\phi}_2(z) du\,du'\,dz.$$

Now the term containing $A(u)$ is equal to

$$\text{(7.31)}\quad \frac{1}{\varepsilon} \int_{\mathbb{R}^{2n}} (A\psi_w^\varepsilon) * G_{\lambda\varepsilon^2}^{(n)}(u' + \varepsilon z) \overline{\psi_w^\varepsilon(u')} \widehat{\phi}_2(z) du'\,dz$$

and the term containing $A(u')$ is equal to

$$\text{(7.32)}\quad \frac{1}{\varepsilon} \int_{\mathbb{R}^{2n}} A(u')\psi_w^\varepsilon * G_{\lambda\varepsilon^2}^{(n)}(u' + \varepsilon z) \overline{\psi_w^\varepsilon(u')} \widehat{\phi}_2(z) du'\,dz.$$

Now subtract (7.32) from (7.31) to get that (7.30) equals $R_{w,1}^\varepsilon + R_{w,2}^\varepsilon$, where

$$R_{w,1}^\varepsilon := \frac{1}{\varepsilon} \int_{\mathbb{R}^{2n}} \left[(A\psi_w^\varepsilon) * G_{\lambda\varepsilon^2}^{(n)}(u' + \varepsilon z) - A(u' + \varepsilon z)\psi_w^\varepsilon * G_{\lambda\varepsilon^2}^{(n)}(u' + \varepsilon z)\right] \overline{\psi_w^\varepsilon(u')} \widehat{\phi}_2(z) du'\,dz$$

and

$$R_{w,2}^\varepsilon := \frac{1}{\varepsilon} \int_{\mathbb{R}^{2n}} [A(u' + \varepsilon z) - A(u')]\psi_w^\varepsilon * G_{\lambda\varepsilon^2}^{(n)}(u' + \varepsilon z) \overline{\psi_w^\varepsilon(u')} \widehat{\phi}_2(z) du'\,dz.$$

Thus, the a priori estimate on the expression in (7.27) can be achieved by estimating the integrals of the error terms $R_{w,i}^\varepsilon$ with respect to w.

Writing $R_{w,1}^\varepsilon$ in the form

$$\int_{\mathbb{R}^n} \widehat{\phi}_2(z) \int_{\mathbb{R}^n \times \mathbb{R}^n} \frac{A(u' + \varepsilon z - u) - A(u' + \varepsilon z)}{\varepsilon} G_{\lambda\varepsilon^2}^{(n)}(u) \overline{\psi_w^\varepsilon(u')} \psi_w^\varepsilon(u' + \varepsilon z - u) du\,du'\,dz,$$

we can estimate from above $\int_W |R^\varepsilon_{w,1}| d\mathbb{P}(w)$ by

$$\|\nabla A\|_\infty \int_W \int_{\mathbb{R}^n} |\hat{\phi}_2|(z) \int_{\mathbb{R}^n\times\mathbb{R}^n} \frac{|u|}{\varepsilon} G^{(n)}_{\lambda\varepsilon^2}(u)|\psi^\varepsilon_w|(u')|\psi^\varepsilon_w|(u'+\varepsilon z-u)du\,du'\,dz\,d\mathbb{P}(w)$$

and then by

$$\sqrt{\lambda}\|\nabla A\|_\infty \int_W \int_{\mathbb{R}^n} |\hat{\phi}_2|(z) \int_{\mathbb{R}^n\times\mathbb{R}^n} \eta_\varepsilon(u)|\psi^\varepsilon_w|(u')|\psi^\varepsilon_w|(u'+\varepsilon z-u)du\,du'\,dz\,d\mathbb{P}(w)$$

where $\eta_\varepsilon(u) := G^{(n)}_{\lambda\varepsilon^2}(u)|u|/(\sqrt{\lambda}\varepsilon)$ is a family of convolution kernels uniformly bounded in L^1 by $\int |u| G^{(n)}_1(u)du$. Using the convolution estimate $\|a * \eta_\varepsilon\|_2 \le \|a\|_2 \,\|\eta_\varepsilon\|_1$, we can finally bound this term with

$$\sqrt{\lambda}\|\nabla A\|_\infty \,\|\hat{\phi}_2\|_1 \int |u| G^{(n)}_1(u)du.$$

We can estimate from above $\int_W |R^\varepsilon_{w,2}| d\mathbb{P}(w)$ using (7.22) to get

$$\sqrt{C(\lambda)} \int_{\mathbb{R}^n} |\hat{\phi}_2|(z) \int_{\mathbb{R}^n} \frac{|A(u'+\varepsilon z) - A(u')|}{\varepsilon} \sqrt{\int_W |\psi^\varepsilon_w|^2(u')d\mathbb{P}(w)}\, du'dz.$$

Then we can use the standard L^2-estimate on difference quotients of $W^{1,2}$-functions to bound this last expression with

$$\sqrt{C(\lambda)}\|\nabla A\|_2 \int_{\mathbb{R}^n} |z|\,|\hat{\phi}_2|(z)dz.$$

This completes the estimate of the term in (7.27) and the proof. □

7.5 Estimates and Convergence of $\mathscr{E}_\varepsilon(U_s, \psi)$

In the case of the Coulomb potential, we follow a specific argument borrowed from [6, proof of theorem 1.1(ii)]), based on the inequality

$$\left|\frac{1}{|z+w/2|} - \frac{1}{|z-w/2|}\right| \le \frac{|w|}{|z+w/2||z-w/2|} \tag{7.33}$$

with $z = (x_\alpha - x_\beta) \in \mathbb{R}^3$, $w = \varepsilon(y_\alpha - y_\beta) \in \mathbb{R}^3$. By estimating the difference quotients of U_s as in (7.33), we obtain

$$\left|\int_{\mathbb{R}^d} \mathscr{E}_\varepsilon(U_s,\psi)\phi\,dx\,dp\right| \le C_* \int_{\mathbb{R}^n} |y| \sup_{x'} |\mathcal{F}_p\phi|(x',y)dy \int_{\mathbb{R}^n} U_s^2|\psi|^2\,dx, \tag{7.34}$$

with C_* depending only on the numbers Z_α in (1.7).

Now we can state the convergence of $\mathscr{E}_\varepsilon(U_s, \psi^\varepsilon)$; the particular form of the statement, with convolution on ϕ on one side and convolution on $W_\varepsilon\psi^\varepsilon$ on the other side (namely the Husimi transform), is motivated by the goal we have in mind, namely the exploitation of the fact that the Husimi transforms asymptotically satisfy the Liouville equation.

THEOREM 7.4 (Convergence of Error Term II) *Let $\psi^\varepsilon \in L^2(\mathbb{R}^n;\mathbb{C})$ be unitary wave functions satisfying*

$$\sup_{\varepsilon>0} \int_{\mathbb{R}^n} U_s^2 |\psi^\varepsilon|^2 \, dx < \infty. \tag{7.35}$$

Then

$$\begin{aligned}\lim_{\varepsilon\to 0} \int_{\mathbb{R}^{2n}} & \mathscr{E}_\varepsilon(U_s,\psi^\varepsilon)\phi * G_\varepsilon^{(n)} \, dx\, dp \\ &+ \int_{\mathbb{R}^{2n}} \langle \nabla U_s, \nabla_p \phi\rangle \widetilde{W}_\varepsilon \psi^\varepsilon \, dx\, dp = 0 \quad \forall \phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S\times\mathbb{R}^n)).\end{aligned} \tag{7.36}$$

PROOF. First of all, we see that we can apply (7.7) with $\varphi = \langle \nabla U_s, \nabla_p \phi\rangle$ to replace the integrals

$$\int_{\mathbb{R}^{2n}} \langle \nabla U_s, \nabla_p \phi\rangle \widetilde{W}_\varepsilon \psi^\varepsilon \, dx\, dp \quad \text{with} \quad \int_{\mathbb{R}^{2n}} \langle \nabla U_s, \nabla_p \phi\rangle W_\varepsilon \psi^\varepsilon \, dx\, dp$$

in the verification of (7.36). Analogously, using (7.35) and (7.34), we see that we can replace

$$\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s,\psi^\varepsilon)\phi * G_\varepsilon^{(n)} \, dx\, dp \quad \text{with} \quad \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s,\psi^\varepsilon)\phi \, dx\, dp.$$

Thus, we are led to show the convergence

$$\begin{aligned}\lim_{\varepsilon\to 0} \int_{\mathbb{R}^{2n}} & \mathscr{E}_\varepsilon(U_s,\psi^\varepsilon)\phi \, dx\, dp \\ &+ \int_{\mathbb{R}^{2n}} \langle \nabla U_s, \nabla_p \phi\rangle W_\varepsilon \psi^\varepsilon \, dx\, dp = 0 \quad \forall \phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S\times\mathbb{R}^n)).\end{aligned} \tag{7.37}$$

Since

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

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 (7.34), with

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

which is infinitesimal, by using (7.35) again, as $\varepsilon \to 0$. Since

$$\frac{U_s(x + \frac{\varepsilon}{2} y) - U_s(x - \frac{\varepsilon}{2} y)}{\varepsilon} \to \langle \nabla U_s(x), y \rangle$$

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 as that of

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

which coincides with

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

□

8 L^∞-Estimates on Averages of ψ

In this section we consider a family of solutions $\psi_{t,w}^\varepsilon$ to the Schrödinger equation (1.1) indexed by a parameter w and derive new estimates on their averages. In particular, we obtain pointwise upper bounds on Husimi transforms.

One of the main advantages of the Husimi transform is that it is nonnegative: indeed, with the change of variables (7.2) and simple computations (see [24] for more details), it can be written as

$$\widetilde{W}_\varepsilon \psi(y, p) = \frac{1}{(2\pi)^n} \langle \rho^\psi \phi_{y,p}^\varepsilon, \phi_{y,p}^\varepsilon \rangle = \frac{1}{(2\pi)^n} |\langle \psi, \phi_{y,p}^\varepsilon \rangle|^2, \tag{8.1}$$

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

$$\phi_{y,p}^\varepsilon(x) := \frac{1}{\varepsilon^{n/2}} \frac{1}{(\pi\varepsilon)^{n/4}} e^{-|x-y|^2/(2\varepsilon)} e^{i(p\cdot x)/\varepsilon} \in L^2(\mathbb{R}^n; \mathbb{C}), \tag{8.2}$$

and $\rho^\psi : L^2(\mathbb{R}^n; \mathbb{C}) \to L^2(\mathbb{R}^n; \mathbb{C})$ is the orthogonal projector onto $\psi \in L^2(\mathbb{R}^n; \mathbb{C})$:

$$[\rho^\psi \phi](x) := \left(\int_{\mathbb{R}^n} \phi(x') \overline{\psi(x')} dx' \right) \psi(x).$$

PROPOSITION 8.1 (L^∞-Estimates) *Let $\psi_w^\varepsilon \in L^2(\mathbb{R}^n; \mathbb{C})$ satisfy the operator inequalities*

$$\frac{1}{\varepsilon^n} \int_W \rho^{\psi_w^\varepsilon} \, d\mathbb{P}(w) \leq C \, \mathrm{Id} \quad \forall \varepsilon > 0.$$

Then

(a) *for all* $y \in \mathbb{R}^n$ *and* $\varepsilon, \lambda > 0$, *we have*

$$\int_W \left|\psi_w^\varepsilon * G_{2\lambda\varepsilon^2}^{(n)}\right|^2(y)\,d\mathbb{P}(w) \le \frac{C}{\lambda^{n/2}};$$

(b) *for all* $(y,p) \in \mathbb{R}^{2n}$ *and* $\varepsilon > 0$, *we have*

$$\int_W \widetilde{W}_\varepsilon \psi_w^\varepsilon(y,p)\,d\mathbb{P}(w) \le C.$$

PROOF. The proof of (a) follows by applying the uniform operator inequality to the functions $(2\varepsilon)^{n/2}(\pi\lambda)^{n/4}G_{2\lambda\varepsilon^2}^{(n)}(\cdot - y)$, whose L^2-norm is 1, to get

$$\varepsilon^n \lambda^{n/2} \int_W \left|\psi_w^\varepsilon * G_{2\lambda\varepsilon^2}^{(n)}\right|^2(y)\,d\mathbb{P}(w) \le C\varepsilon^n.$$

The proof of (b) is analogous; it is based on (8.1) and on the insertion of the functions $\phi_{y,p}^\varepsilon$ in (8.2) in the operator inequality, taking into account that $\|\phi_{y,p}^\varepsilon\|_2 = \varepsilon^{-n/2}$. □

The assumption made in Proposition 8.1 is compatible with the families of wave functions given in (1.17), i.e.,

$$\psi_w^\varepsilon(x) = \varepsilon^{-n\alpha/2}\phi_0\left(\frac{x - x_0}{\varepsilon^\alpha}\right)e^{i(x\cdot p_0)/\varepsilon}, \quad \phi_0 \in C_c^2(\mathbb{R}^n),\ 0 < \alpha < 1, \tag{8.3}$$

with $w = (x_0, p_0)$. Indeed, in this case one can choose $W = \mathbb{R}^{2n}$ with the Borel σ-algebra and $\mathbb{P} = \rho\mathscr{L}^{2n}$, with $\rho \in L^1 \cap L^\infty$; see [17] for details. In the extreme case $\alpha = 1$ no average with respect to p_0 is needed and one can fix it and choose $W = \mathbb{R}^n$, obtaining convergence for almost all x_0, so to speak. The other extreme case $\alpha = 0$, corresponding to concentration in momentum, is analogous.

9 Main Convergence Result

In this section we combine the theory developed in Sections 2 through 6 with the estimates of Sections 7 and 8 to obtain convergence of the Wigner-Husimi transforms of solutions to (1.1). In particular, we shall apply Theorem 5.2.

We consider the assumptions on U stated in Section 7.2 and "random" initial data $\psi_{0,w}^\varepsilon \in H^2(\mathbb{R}^n;\mathbb{C})$ with unit L^2-norm in (1.1) indexed by $w \in W$, where $(W, \mathcal{F}, \mathbb{P})$ is a suitable probability space. Denoting by $\psi_{t,w}^\varepsilon$ the corresponding

Schrödinger evolutions, the basic assumptions we need for the initial data are

$$\begin{gathered}\sup_{\varepsilon>0}\int_W\int_{\mathbb{R}^n}|H_\varepsilon\psi^\varepsilon_{0,w}|^2\,dx\,d\mathbb{P}(w)<\infty,\\ \lim_{R\uparrow\infty}\sup_{\varepsilon>0}\int_W\int_{\mathbb{R}^n\setminus B_R}|\psi^\varepsilon_{0,w}|^2\,dx\,d\mathbb{P}(w)=0;\end{gathered}\tag{9.1}$$

$$\frac{1}{\varepsilon^n}\int_W\rho^{\psi^\varepsilon_{0,w}}\,d\mathbb{P}(w)\le C\,\mathrm{Id}\quad\text{with } C \text{ independent of } \varepsilon;\tag{9.2}$$

$$i(w):=\lim_{\varepsilon\downarrow 0}\widetilde{W}_\varepsilon\psi^\varepsilon_{0,w}\mathscr{L}^d\quad\text{exists in } \mathscr{P}(\mathbb{R}^d) \text{ for } \mathbb{P}\text{-a.e. } w\in W.\tag{9.3}$$

As we discussed in the introduction and in Section 8, the assumptions (9.1), (9.2), and (9.3) are compatible with several natural families of initial conditions; see, for instance, (1.17) or (8.3). In addition, the unitary character of the Schrödinger evolution immediately gives

$$\frac{1}{\varepsilon^n}\int_W\rho^{\psi^\varepsilon_{t,w}}\,d\mathbb{P}(w)\le C\,\mathrm{Id}\quad\forall\varepsilon>0,\ t\ge 0,\tag{9.4}$$

where C is the same constant as in (9.2).

In the next theorem we state our convergence result first in terms of the Husimi transforms (see (9.5) below), where $d_{\mathscr{P}}$ is any bounded distance inducing the topology of $\mathscr{P}(\mathbb{R}^{2n})$. Choosing $\{\varphi_k\}\subset C^\infty_c(\mathbb{R}^{2n})$ suitable for (7.8), we then obtain the convergence result in terms of Wigner transforms.

THEOREM 9.1 *For U as in Section* 7.2*, and under assumptions* (9.1), (9.2)*, and* (9.3)*, we have*

$$\lim_{\varepsilon\to 0}\int_W\sup_{t\in[-T,T]}d_{\mathscr{P}}(\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w},\boldsymbol{\mu}(t,i(w)))\,d\mathbb{P}(w)=0\tag{9.5}$$

for all $T>0$, where $\boldsymbol{\mu}(t,\mu)$ is the $\boldsymbol{\nu}$-RLF in (6.3) *for $\boldsymbol{\nu}=i_\sharp\mathbb{P}\in\mathscr{P}(\mathscr{P}(\mathbb{R}^{2n}))$. In addition, choosing $d_{\mathcal{A}'}$ as in* (7.8)*, we have*

$$\lim_{\varepsilon\to 0}\int_W\sup_{t\in[-T,T]}d_{\mathcal{A}'}\big(W_\varepsilon\psi^\varepsilon_{t,w},\boldsymbol{\mu}(t,i(w))\big)d\mathbb{P}(w)=0.\tag{9.6}$$

PROOF. Our goal is to apply Theorem 5.2 (with a continuous parameter ε) and Remark 5.3 with $i_\varepsilon(w):=\widetilde{W}_\varepsilon\psi^\varepsilon_{0,w}\mathscr{L}^{2n}$ and $\boldsymbol{\mu}_\varepsilon(t,i_\varepsilon(w))=\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\mathscr{L}^{2n}$. The convergence (9.5) will be a direct consequence of (5.3). We shall work in the time interval $[0,T]$, the proof in the time interval $[-T,0]$ being the same, up to a time reversal.

First of all, we notice that (9.1) and (7.17) give

$$\sup_{\varepsilon>0}\sup_{t\in\mathbb{R}}\int_W\int_{\mathbb{R}^n}|H_\varepsilon\psi^\varepsilon_{t,w}|^2\,dx\,d\mathbb{P}(w)<\infty. \tag{9.7}$$

In particular, by an integration by parts, we also have

$$\sup_{\varepsilon>0}\sup_{t\in\mathbb{R}}\int_W\int_{\mathbb{R}^n}|\varepsilon\nabla\psi^\varepsilon_{t,w}|^2\,dx\,d\mathbb{P}(w)<\infty. \tag{9.8}$$

(1) ASYMPTOTIC REGULARITY. By (9.4) and Proposition 8.1(b) we have the uniform estimate (in ε, t, and (x,p))

$$\int_W \widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}(x,p)d\mathbb{P}(w)\le C. \tag{9.9}$$

In particular, we have uniform and not only asymptotic regularity; therefore Remark 5.3 applies.

(2) UNIFORM DECAY AWAY FROM THE SINGULARITY. We check (5.1) with $\beta=2$ and S equal to the singular set of U_s, namely,

$$\sup_{\delta>0}\limsup_{\varepsilon\to0}\int_W\int_0^T\int_{B_R}\frac{1}{\operatorname{dist}^2(x,S)+\delta}\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp\,dt\,d\mathbb{P}(w)<\infty. \tag{9.10}$$

We use (7.3) and the inequality

$$\frac{1}{\operatorname{dist}^2(x,S)+\delta}*G^{(n)}_\varepsilon\le\frac{1}{\operatorname{dist}^2(x,S)},$$

which holds in B_R for $\varepsilon<\varepsilon(\delta,R)$ to deduce (9.10) from

$$\limsup_{\varepsilon\to0}\int_W\int_0^T\int_{\mathbb{R}^n}\frac{1}{\operatorname{dist}^2(x,S)}|\psi^\varepsilon_{t,w}|^2\,dx\,dt\,d\mathbb{P}(w)<\infty. \tag{9.11}$$

In turn, this inequality follows by (7.18) and (7.15), taking (9.1) into account.

(3) SPACE TIGHTNESS. We have to check that for all $\delta>0$ the following holds:

$$\lim_{R\to\infty}\mathbb{P}\left(\left\{w\in W:\sup_{\varepsilon>0}\sup_{t\in[0,T]}\int_{\mathbb{R}^{2n}\setminus B_R}\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp>\delta\right\}\right)=0.$$

Considering the cube C_R containing B_R, this tightness property can be checked separately for the first and the second marginals of $\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}$; using (7.3) and (7.4), it is not hard to see that it suffices to check the analogous property for the marginals of the corresponding Wigner transforms; for the first marginals, tightness is a direct consequence of (7.19) and (9.1). For the second marginals, we use (9.8) and the identity

$$\int_{\mathbb{R}^n\times\mathbb{R}^n} |p|^2 W_\varepsilon\psi\,dx\,dp = \int_{\mathbb{R}^n} \left|\frac{1}{(2\pi\varepsilon)^{n/2}}\widehat{\psi}(p/\varepsilon)\right|^2 |p|^2\,dp = \int_{\mathbb{R}^n} |\varepsilon\nabla\psi|^2\,dx \tag{9.12}$$

with $\psi = \psi^\varepsilon_{t,w}$.

(4) TIME TIGHTNESS. We need to show that for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$ the following holds:

$$\lim_{M\uparrow\infty} \mathbb{P}\left(\left\{w\in W : \int_0^T \left|\left(\int_{\mathbb{R}^{2n}} \phi\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp\right)'\right|dt > M\right\}\right) = 0$$

uniformly in ε. Equivalently, we can consider the limit

$$\lim_{M\uparrow\infty} \mathbb{P}\left(\left\{w\in W : \int_0^T \left|\left(\int_{\mathbb{R}^{2n}} \phi_\varepsilon W_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp\right)'\right|dt > M\right\}\right) = 0, \tag{9.13}$$

where $\phi_\varepsilon = \phi * G_\varepsilon^{(2n)}$. According to (1.13), the time derivative in the formula above consists of two terms,

$$\int \langle p, \nabla_x\phi_\varepsilon\rangle W_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp \quad \text{and} \quad \int \mathscr{E}_\varepsilon(U, \psi^\varepsilon_{t,w})\phi_\varepsilon\,dx\,dp,$$

and we need only to show a property analogous to (9.13) for these two terms. Since $\phi \in C_c^\infty(\mathbb{R}^{2n})$, $\|\langle p, \nabla_x\phi_\varepsilon\rangle\|_{\mathcal{A}}$ are easily seen to be uniformly bounded; hence the first term can be estimated using (7.6). The second term can be estimated using (7.20) for U_b and (7.34) for U_s, taking (7.18) and (9.1) into account.

(5) LIMIT CONTINUITY EQUATION. We have to show that

$$\lim_{\varepsilon\downarrow 0}\int_W \left|\int_0^T \left[\varphi'(t)\int_{\mathbb{R}^{2n}} \phi\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp + \varphi(t)\int_{\mathbb{R}^{2n}} \langle \boldsymbol{b}, \nabla\phi\rangle\widetilde{W}_\varepsilon\psi^\varepsilon_{t,w}\,dx\,dp\right]dt\right| d\mathbb{P}(w) = 0$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n))$, $\varphi \in C_c^\infty(0,T)$. Taking (7.9) into account, this is implied by the validity of the limits

$$\lim_{\varepsilon \downarrow 0} \sup_{t \in [0,T]} \int_W \Bigg| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U, \psi^\varepsilon_{t,w}) \phi * G_\varepsilon^{(2n)}\, dx\, dp + \int_{\mathbb{R}^{2n}} \langle \nabla U, \nabla_p \phi \rangle \widetilde{W}_\varepsilon \psi^\varepsilon_{t,w}\, dx\, dp \Bigg| d\mathbb{P}(w) = 0, \tag{9.14}$$

$$\lim_{\varepsilon \downarrow 0} \sqrt{\varepsilon} \int_W \int_0^T |\varphi(t)| \Bigg| \int_{\mathbb{R}^{2n}} \phi \nabla_x \cdot [W_\varepsilon \psi^\varepsilon_{t,w} * \overline{G}_\varepsilon^{(2n)}] dx\, dp \Bigg| dt\, d\mathbb{P}(w) = 0. \tag{9.15}$$

VERIFICATION OF (9.14). We can consider separately the contributions of U_b and U_s. For the U_b contribution we apply Theorem 7.2 in the form stated in (7.24); assumptions (7.21) and (7.22) of that theorem are fulfilled in view of (9.2) and Proposition 8.1. For the U_s contribution, we apply (7.36) of Theorem 7.4; assumption (7.35) of that theorem is fulfilled in view of assumption (9.1) on the initial data and (7.18), ensuring propagation in time.

VERIFICATION OF (9.15). This is easy, taking into account the fact that

$$\int_{\mathbb{R}^{2n}} \langle W_\varepsilon \psi^\varepsilon_{t,w} * \overline{G}_\varepsilon^{(2n)}, \nabla_x \phi \rangle dx\, dp = - \int_{\mathbb{R}^{2n}} W_\varepsilon \psi^\varepsilon_{t,w} \nabla_x \cdot [\phi * \overline{G}_\varepsilon^{(2n)}] dx\, dp$$

are uniformly bounded because $\overline{G}_\varepsilon^{(2n)}$, defined in (7.10), are uniformly bounded in $L^1(\mathbb{R}^n)$.

DEDUCTION OF (9.6) FROM (9.5). Let $\{\varphi_k\}_{k \geq 1}$ as in (7.8). Since

$$d'_{\mathscr{P}}(\mu, \nu) := d_{\mathscr{P}}(\mu, \nu) + \min\left\{ \left| \int_{\mathbb{R}^{2n}} \varphi_k\, d(\mu - \nu) \right|, 1 \right\}$$

is still a bounded distance inducing the topology of $\mathscr{P}(\mathbb{R}^{2n})$, for any $k \geq 1$ we infer from (9.5)

$$\lim_{\varepsilon \to 0} \int_W \sup_{t \in [-T,T]} \left| \int_{\mathbb{R}^{2n}} \varphi_k d(\widetilde{W}_\varepsilon \psi^\varepsilon_{t,w} - \boldsymbol{\mu}(t, i(w))) \right| d\mathbb{P}(w) = 0.$$

Taking (7.7) into account, this gives

$$\lim_{\varepsilon \to 0} \int_W \sup_{t \in [-T,T]} \left| \int_{\mathbb{R}^{2n}} \varphi_k d(W_\varepsilon \psi^\varepsilon_{t,w} - \boldsymbol{\mu}(t, i(w))) \right| d\mathbb{P}(w) = 0.$$

Since k is arbitrary, the definition of $d_{\mathcal{A}'}$ gives (9.6). □

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