arXiv:1209.3903v2 [math.NA] 17 Sep 2013

ON FOURIER TIME-SPLITTING METHODS FOR NONLINEAR SCHRÖDINGER EQUATIONS IN THE SEMI-CLASSICAL LIMIT

RÉMI CARLES

Abstract. We prove an error estimate for a Lie-Trotter splitting operator associated to the Schrödinger-Poisson equation in the semiclassical regime, when the WKB approximation is valid. In finite time, and so long as the solution to a compressible Euler-Poisson equation is smooth, the error between the numerical solution and the exact solution is controlled in Sobolev spaces, in a suitable phase/amplitude representation. As a corollary, we infer the numerical convergence of the quadratic observables with a time step independent of the Planck constant. A similar result is established for the nonlinear Schrödinger equation in the weakly nonlinear regime.

1. Introduction

We consider the nonlinear Schrödinger equation, for $t \geqslant 0$,

$$i\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\Delta u^\varepsilon = \varepsilon^\alpha f\left(|u^\varepsilon|^2\right)u^\varepsilon. \tag{1.1}$$

The function $u^\varepsilon = u^\varepsilon(t,x)$ is complex-valued, and the space variable x belongs to $\mathbf{R}^d$. The presence of the parameter ε is motivated by the *semi-classical limit*, $\varepsilon \to 0$. Physically, ε corresponds to a small ratio between microscopic and macroscopic quantities, so the limit $\varepsilon \to 0$ is expected to yield a relevant approximation; see e.g. [18] and references therein. The parameter $\alpha \geqslant 0$ measures the strength of nonlinear interactions: in the WKB regime, which is recalled below, the nonlinearity is negligible if $\alpha > 1$, it has a leading order (moderate) influence if $\alpha = 1$ (weakly nonlinear regime), and its influence is very strong in the regime $\varepsilon \to 0$ if $\alpha = 0$. The case $0 < \alpha < 1$ is not considered here, but it should be considered as similar to the case $\alpha = 0$ ([7]).

In this paper, we consider mostly two families of nonlinearity:

- Nonlocal nonlinearity in the case $\alpha = 0$: $f(\rho) = K * \rho$.
- Local or nonlocal nonlinearity in the case $\alpha \geqslant 1$.

The first case includes the Schrödinger-Poisson system in space dimension $d \geqslant 3$ ($f(\rho) = \lambda\Delta^{-1}\rho$, $\lambda \in \mathbf{R}$, hence $K(x) = \lambda c_d/|x|^{d-2}$). The second case includes the cubic nonlinearity (focusing or defocusing). We will also discuss why the case of the cubic nonlinearity is not treated in the regime $\alpha = 0$ (see Remark 6.3). Our analysis is limited to bounded time intervals, so the exponentials are controlled, which is the reason why we do not keep track of such factors when they are eventually included in a uniform constant. The reason why the analysis is bound to finite time intervals is, in the case $\alpha = 0$, that the solution of the Euler-Poisson equation generically

---

This work was supported by the French ANR projects BECASIM (ANR-12-MONU-0007-04) and SchEq (ANR-12-JS01-0005-01).

develops a singularity in finite time, and, in the case $\alpha \geqslant 1$, that the solution of the Burgers' equation generically develops a singularity in finite time.

The initial data that we consider are of WKB type:

$$u^\varepsilon(0,x) = a_0(x) e^{i\phi_0(x)/\varepsilon}. \tag{1.2}$$

An important well-known property of this framework is related to the following quantities (quadratic observables),

$$\begin{aligned} \text{Position density: } & \rho^\varepsilon(t,x) = |u^\varepsilon(t,x)|^2. \\ \text{Current density: } & J^\varepsilon(t,x) = \varepsilon \operatorname{Im}\left(\overline{u}^\varepsilon(t,x)\nabla u^\varepsilon(t,x)\right). \end{aligned}$$

Consider the case of Schrödinger-Poisson system in dimension $d \geqslant 3$, with $\alpha = 0$. Formally, ρ^ε and J^ε converge to the solution of the compressible Euler-Poisson equation

$$\begin{cases} \partial_t \rho + \operatorname{div} J = 0; \quad \rho_{|t=0} = |a_0|^2, \\ \partial_t J + \operatorname{div}\left(\dfrac{J\otimes J}{\rho}\right) + \rho\nabla P = 0; \quad J_{|t=0} = |a_0|^2 \nabla\phi_0, \\ \Delta P = \lambda\rho, \quad P(t,x), \nabla P(t,x) \to 0 \text{ as } |x| \to \infty. \end{cases} \tag{1.3}$$

See e.g. [6, 27] for a rigorous statement of this result.

1.1. **Fourier time-splitting methods.** When simulating numerically (1.1), the size of ε becomes an important parameter: if the nonlinearity f is replaced by an external potential $V(x)$ (independent of u^ε), then it was proved in [23] that finite difference approximation requires to consider a time step $\Delta t = o(\varepsilon)$ in order to recover the above quadratic observables. In [3], it was proved that these quadratic observables can be accurately recovered for time steps independent of ε, if time splitting methods are considered and V is bounded as well as all its derivatives. Moreover, if $\Delta t = o(\varepsilon)$, then the wave function u^ε itself is well approximated; see also [12, Theorem 2]. In the appendix, we extend this result to the case of unbounded potentials, which grow at most quadratically in space.

In the nonlinear framework (1.1), numerical experiences in [4] suggest that considering $\Delta t = \mathcal{O}(\varepsilon)$ is enough to recover the correct observables for time splitting spectral methods, when $\alpha = 1$, or $\alpha = 0$ with a defocusing nonlinearity. In the references mentioned so far, space discretization is considered too: in the present paper, we shall discuss only the time discretization, hence the above restrictions. In the recent paper [13], some precise local error estimates have been established, showing that the assumption $\Delta t = \mathcal{O}(\varepsilon)$ is a sensible assumption for the local error to behave properly. We underscore that if crucial, the local error estimate is not sufficient to obtain a global error estimate, unlike in [22], because of rapid oscillations.

We now briefly recall what time splitting methods consist in, in the context of (1.1). The remark is that if the Laplacian or the nonlinearity is discarded in (1.1), then the equation becomes explicitly solvable. We denote by X^t_ε the map $v^\varepsilon(0,\cdot) \mapsto v^\varepsilon(t,\cdot)$, where

$$i\varepsilon\partial_t v^\varepsilon + \frac{\varepsilon^2}{2}\Delta v^\varepsilon = 0. \tag{1.4}$$

The above equation is solved explicitly by using the Fourier transform (defined in Assumption 1.2 below), since it becomes an ordinary differential equation

$$i\varepsilon\partial_t\widehat{v}^\varepsilon - \frac{\varepsilon^2}{2}|\xi|^2\widehat{v}^\varepsilon = 0, \tag{1.5}$$

hence

$$\widehat{X_\varepsilon^t v}(\xi) = e^{-i\varepsilon\frac{t}{2}|\xi|^2}\widehat{v}(\xi).$$

If we now denote by Y_ε^t the map $w^\varepsilon(0,\cdot)\mapsto w^\varepsilon(t,\cdot)$, where

$$i\varepsilon\partial_t w^\varepsilon = \varepsilon^\alpha f\left(|w^\varepsilon|^2\right)w^\varepsilon, \tag{1.6}$$

then we remark that since f is real-valued, the modulus of w^ε does not depend on time, hence

$$Y_\varepsilon^t w(x) = w(x)e^{-i\varepsilon^\alpha\frac{t}{\varepsilon}f(|w(x)|^2)}. \tag{1.7}$$

At this stage, it is already clear that whether $\alpha \geqslant 1$ or $\alpha < 1$, the estimates for Y_ε^t will be rather different. We shall denote by S_ε^t the nonlinear flow associated to (1.1): $S_\varepsilon^t u^\varepsilon(0,\cdot) = u^\varepsilon(t,\cdot)$.

We consider the Lie-type splitting operator

$$Z_\varepsilon^t = Y_\varepsilon^t X_\varepsilon^t, \tag{1.8}$$

for which calculations will be less involved than for the Strang-type splitting operator

$$Z_{\varepsilon,S}^t = X_\varepsilon^{t/2}Y_\varepsilon^t X_\varepsilon^{t/2}.$$

Since both X_ε^t and Y_ε^t are unitary on L^2, so is Z_ε^t:

$$\|X_\varepsilon^t\|_{L^2\to L^2} = \|Y_\varepsilon^t\|_{L^2\to L^2} = \|Z_\varepsilon^t\|_{L^2\to L^2} = 1. \tag{1.9}$$

The action of Z_ε^t on Sobolev spaces is more involved, because of the nonlinear operator Y_ε^t (in the case $\alpha = 0$). In the case $\varepsilon = 1$ with $f(y) = y$ (cubic nonlinearity), the convergence of the approximate solution generated by the splitting operator as the time step goes to zero has been established in [5] for $x \in \mathbf{R}^d$, $d \leqslant 2$, and in [22] for $x \in \mathbf{R}^3$.

Theorem 1.1 (From [5, 22])**.** *Let* $\varepsilon = 1$, $f(y) = y$, *and* $d \leqslant 2$. *For all* $u_0 = u^\varepsilon_{|t=0} \in H^2(\mathbf{R}^d)$ *and all* $T > 0$, *there exist* C *and* h_0 *such that for all* $\Delta t \in (0, h_0]$, *for all* $n \in \mathbf{N}$ *such that* $n\Delta t \in [0,T]$,

$$\left\|\left(Z_1^{\Delta t}\right)^n u_0 - S^{n\Delta t}u_0\right\|_{L^2} \leqslant C\left(m_2, T\right)\Delta t,$$

where, for $j \in \mathbf{N}$,

$$m_j = \max_{0\leqslant t\leqslant T}\|u(t)\|_{H^j(\mathbf{R}^d)}.$$

If $d = 3$ *and* $u_0 \in H^4(\mathbf{R}^d)$, *then*

$$\left\|\left(Z_{1,S}^{\Delta t}\right)^n u_0 - S^{n\Delta t}u_0\right\|_{L^2} \leqslant C\left(m_4, T\right)(\Delta t)^2.$$

Note however that these results do not directly yield interesting information in the case of (1.1) in the semi-classical limit: in the presence of rapid oscillations as in (1.1), the quantity m_j behaves like ε^{-j}, so the bounds in [5, 22] cease to be interesting.

On a more technical level, note that even though Z_ε^t is unitary on L^2, a standard Lady Windermere's fan argument, which consists in writing

$$u_n - u(t_n) = \sum_{j=0}^{n-1} \left(\left(Z_\varepsilon^{\Delta t}\right)^{n-j-1} Z_\varepsilon^{\Delta t} S_\varepsilon^{j\Delta t} u_0 - \left(Z_\varepsilon^{\Delta t}\right)^{n-j-1} S_\varepsilon^{\Delta t} S_\varepsilon^{j\Delta t} u_0 \right), \tag{1.10}$$

cannot be used directly, since Z_ε^t is not a linear operator. Therefore, nonlinear estimates are needed. Eventually, a Lady Windermere's fan argument different from (1.10) is used. In the case of the Schrödinger-Poisson system, the proof in [22] uses for instance the estimate

$$\|\Delta^{-1}(uv)w\|_{L^2(\mathbf{R}^3)} \leqslant C\|u\|_{H^1(\mathbf{R}^3)}\|v\|_{L^2(\mathbf{R}^3)}\|w\|_{L^2(\mathbf{R}^3)}.$$

In the present framework, functions are ε-oscillatory (see Remark 1.4 below), so the natural adaptation of the above estimates is of the form

$$\|\Delta^{-1}(u^\varepsilon v^\varepsilon)w^\varepsilon\|_{L^2(\mathbf{R}^3)} \leqslant C\varepsilon^{-1/2}\|u^\varepsilon\|_{H^1_\varepsilon(\mathbf{R}^3)}\|v^\varepsilon\|_{L^2(\mathbf{R}^3)}\|w^\varepsilon\|_{L^2(\mathbf{R}^3)},$$

where C is independent of ε and

$$\|u^\varepsilon\|_{H^1_\varepsilon(\mathbf{R}^3)} = \sup_{0<\varepsilon\leqslant 1}\left(\|u^\varepsilon\|_{L^2} + \|\varepsilon\nabla u^\varepsilon\|_{L^2}\right)$$

is expected to be bounded uniformly in ε, unlike the standard H^1-norm. We then face an $\varepsilon^{-1/2}$ singular factor in the above estimate, which ruins the approach of [22] in the semi-classical limit. Such phenomena explain why there is a gap between the proof in the semi-classical regime for the *linear* Schrödinger equation [12] and adapting the arguments of [22] to the semi-classical regime, even with the local error estimate of [13].

1.2. **WKB analysis.**

Given (1.1) with initial datum (1.2), WKB method consists in seeking

$$u^\varepsilon(t,x) = a^\varepsilon(t,x)e^{i\phi(t,x)/\varepsilon}, \quad \text{with } a^\varepsilon \approx a + \varepsilon a^{(1)} + \dots$$

Plugging this ansatz into (1.1) and ordering the powers of ε, we find formally:

$$\mathcal{O}(\varepsilon^0): \quad \partial_t\phi + \frac{1}{2}|\nabla\phi|^2 = \begin{cases} 0 & \text{if } \alpha \geqslant 1, \\ -f\left(|a|^2\right) & \text{if } \alpha = 0. \end{cases}$$

$$\mathcal{O}(\varepsilon^1): \quad \partial_t a + \nabla\phi\cdot\nabla a + \frac{1}{2}a\Delta\phi = \begin{cases} 0 & \text{if } \alpha > 1, \\ -if\left(|a|^2\right)a & \text{if } \alpha = 1, \\ -2if'\left(|a|^2\right)a\operatorname{Re}\left(\overline{a}a^{(1)}\right) & \text{if } \alpha = 0. \end{cases}$$

We see that if $\alpha > 1$, then the nonlinearity does not affect the pair (a,ϕ), which describes the behavior of u^ε at leading order. On the other hand, if $\alpha = 1$, the transport equation for a is nonlinear, while the equation for ϕ is the same as in the linear case: one speaks of *weakly nonlinear* regime. Finally, in the case $\alpha = 0$, the system of equations shows a strong coupling between all the terms, and is actually not even closed.

In the rest of this subsection, we focus our attention on the case $\alpha = 0$. An important remark consists in noticing that the transport equation

$$\partial_t a + \nabla\phi\cdot\nabla a + \frac{1}{2}a\Delta\phi = -2if'\left(|a|^2\right)a\operatorname{Re}\left(\overline{a}a^{(1)}\right), \tag{1.11}$$

enjoys the following property: even though it cannot be solved when $a^{(1)}$ is unknown, it is of the form $D_t a = ia \times \mathbf{R}$, where D_t stands for the vector field $\partial_t + \nabla\phi \cdot \nabla + \frac{1}{2}\Delta\phi$. Therefore, $D_t|a|^2 = 0$, and if we set $(v,\rho) = (\nabla\phi, |a|^2)$, then the system in (ϕ, a) becomes the closed system

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho v) = 0; \quad \rho_{|t=0} = |a_0|^2, \\ \partial_t v + v\cdot\nabla v + \nabla f(\rho) = 0; \quad v_{|t=0} = \nabla\phi_0. \end{cases} \tag{1.12}$$

Note also that if we set $\tilde{J} = \rho v$, then $(\rho, \tilde{J})$ solves (1.3): we have written (1.3) in a different form, which is also encountered in fluids mechanics. As a matter of fact, in the case of a nonlocal nonlinearity $f(\rho) = K * \rho$, (1.11) is not correct, but since this term has disappeared in (1.12), we do not write the correct version of (1.11), which is a bit involved to present. In the case of a nonlocal nonlinearity, we will make the following assumption.

Assumption 1.2. *The nonlinearity f is of the form $f(\rho) = K*\rho$, where the kernel K is such that its Fourier transform, defined by*

$$\widehat{K}(\xi) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbf{R}^d} e^{-ix\cdot\xi} K(x)dx,$$

satisfies:

- *If $d \leqslant 2$,*
$$\sup_{\xi\in\mathbf{R}^d} (1+|\xi|^2)|\widehat{K}(\xi)| < \infty.$$
- *If $d \geqslant 3$,*
$$\sup_{\xi\in\mathbf{R}^d} |\xi|^2|\widehat{K}(\xi)| < \infty.$$

Typically, this includes the case of Schrödinger-Poisson system if $d \geqslant 3$, where $f(\rho)$ is given by the Poisson equation

$$\Delta f = \lambda\rho, \quad f, \nabla f \to 0 \text{ as } |x| \to \infty,$$

with $\lambda \in \mathbf{R}$. This equation can be solved by Fourier analysis if $d \geqslant 3$ ($\widehat{K}(\xi) = -\lambda|\xi|^{-2}$); if $d \leqslant 2$, this is no longer the case, as discussed in [24]. Under this assumption, (1.12) has a unique solution $(v,\rho) \in C([0,T]; H^{s+1} \times (H^s \cap L^1))$ provided that the initial data are sufficiently smooth, with $s > d/2+1$, from [15] (see also [1, 20, 27], and Section 3 for the main steps of the proof).

Proposition 1.3. *Suppose that f satisfies Assumption 1.2. Let $a_0, \phi_0 \in \mathcal{S}'(\mathbf{R}^d)$ with $(\nabla\phi_0, a_0) \in H^{s+1} \times H^s$ for some $s > d/2$. There exists a unique maximal solution $(v,\rho) \in C\left([0,T_{\max}); H^{s+1} \times (H^s \cap L^1)\right)$ to (1.12). In addition, $T_{\max}$ is independent of $s > d/2+1$ and*

$$T_{\max} < +\infty \Longrightarrow \int_0^{T_{\max}} \left(\|v(t)\|_{W^{1,\infty}} + \|a(t)\|_{W^{1,\infty}}\right) dt = +\infty.$$

Remark 1.4. We note from (1.12) that even if no rapid oscillation is present initially in (1.2), then $v_{|t=0} = 0$ and $\partial_t v_{|t=0} \neq 0$, so the solution u^ε is not ε-oscillatory at time $t = 0$, but becomes *instantaneously* ε-oscillatory.

We emphasize the fact that under Assumption 1.2, and for fixed $\varepsilon > 0$, given $u_0^\varepsilon \in L^2(\mathbf{R}^d)$, (1.1) has a unique, global solution $u^\varepsilon \in C([0,\infty); L^2)$. Moreover, higher Sobolev regularity is propagated globally in time (the nonlinearity is L^2-subcritical); see e.g. [10].

1.3. **Main results.** Our main result measures the accuracy of the time splitting operator so long as the solution to (1.12) remains smooth.

Theorem 1.5. *Suppose that $d \geqslant 1$, $\alpha = 0$ in (1.1), and that f satisfies Assumption 1.2. Let $(\phi_0, a_0) \in L^\infty(\mathbf{R}^d) \times H^s(\mathbf{R}^d)$ with $s > d/2 + 2$, and such that $\nabla\phi_0 \in H^{s+1}(\mathbf{R}^d)$. Let $T > 0$ be such that the solution to (1.12) satisfies $(v, \rho) \in C([0,T]; H^{s+1} \times H^s)$. Consider $u^\varepsilon = S^t_\varepsilon u^\varepsilon_0$ solution to (1.1) and u^ε_0 given by (1.2). There exist $\varepsilon_0 > 0$ and C, c_0 independent of $\varepsilon \in (0, \varepsilon_0]$ such that for all $\Delta t \in (0, c_0]$, for all $n \in \mathbf{N}$ such that $t_n = n\Delta t \in [0,T]$, the following holds:*
1. There exist ϕ^ε and a^ε with

$$\sup_{t\in[0,T]} \left(\|a^\varepsilon(t)\|_{H^s(\mathbf{R}^d)} + \|\nabla\phi^\varepsilon(t)\|_{H^{s+1}(\mathbf{R}^d)} + \|\phi^\varepsilon(t)\|_{L^\infty(\mathbf{R}^d)} \right) \leqslant C, \quad \forall \varepsilon \in (0, \varepsilon_0],$$

such that $u^\varepsilon(t,x) = a^\varepsilon(t,x) e^{i\phi^\varepsilon(t,x)/\varepsilon}$ for all $(t,x) \in [0,T] \times \mathbf{R}^d$.
2. There exist ϕ^ε_n and a^ε_n with

$$\|a^\varepsilon_n\|_{H^s(\mathbf{R}^d)} + \|\nabla\phi^\varepsilon_n\|_{H^{s+1}(\mathbf{R}^d)} + \|\phi^\varepsilon_n\|_{L^\infty(\mathbf{R}^d)} \leqslant C, \quad \forall \varepsilon \in (0, \varepsilon_0],$$

such that $(Z^{\Delta t}_\varepsilon)^n \left(a_0 e^{i\phi_0/\varepsilon} \right) = a^\varepsilon_n e^{i\phi_n/\varepsilon}$, and the following error estimate holds:

$$\|a^\varepsilon_n - a^\varepsilon(t_n)\|_{H^{s-1}} + \|\nabla\phi^\varepsilon_n - \nabla\phi^\varepsilon(t_n)\|_{H^s} + \|\phi^\varepsilon_n - \phi^\varepsilon(t_n)\|_{L^\infty} \leqslant C\Delta t.$$

Note that in the above result, the phase/amplitude representation of the exact solution u^ε and the numerical solution is not unique. This result shows in particular that the splitting solution remains bounded in L^∞, uniformly in ε, in the WKB regime. We infer the convergence of the wave functions in L^2, by reconstructing the numerical wave function:

Corollary 1.6. *Under the assumptions of Theorem 1.5, there exist $\varepsilon_0 > 0$ and C, c_0 independent of $\varepsilon \in (0, \varepsilon_0]$ such that for all $\Delta t \in (0, c_0]$, for all $n \in \mathbf{N}$ such that $n\Delta t \in [0,T]$,*

$$\left\| (Z^{\Delta t}_\varepsilon)^n u^\varepsilon_0 - S^{t_n}_\varepsilon u^\varepsilon_0 \right\|_{L^2(\mathbf{R}^d)} \leqslant C \frac{\Delta t}{\varepsilon}.$$

We also get the convergence of the main quadratic observables:

Corollary 1.7. *Under the assumptions of Theorem 1.5, there exist $\varepsilon_0 > 0$ and C, c_0 independent of $\varepsilon \in (0, \varepsilon_0]$ such that for all $\Delta t \in (0, c_0]$, for all $n \in \mathbf{N}$ such that $n\Delta t \in [0,T]$,*

$$\begin{aligned} &\left\| \left| (Z^{\Delta t}_\varepsilon)^n u^\varepsilon_0 \right|^2 - |\rho^\varepsilon(t_n)|^2 \right\|_{L^1(\mathbf{R}^d)\cap L^\infty(\mathbf{R}^d)} \leqslant C\Delta t, \\ &\left\| \operatorname{Im}\left(\varepsilon \overline{(Z^{\Delta t}_\varepsilon)^n u^\varepsilon_0} \nabla (Z^{\Delta t}_\varepsilon)^n u^\varepsilon_0 \right) - J^\varepsilon(t_n) \right\|_{L^1(\mathbf{R}^d)\cap L^\infty(\mathbf{R}^d)} \leqslant C\Delta t. \end{aligned}$$

These results may seem limited, inasmuch as they address only a specific regime, and say nothing on the large time behavior. We emphasize the fact that the behavior of u^ε as $\varepsilon \to 0$ at time where the solution to (1.12) ceases to be smooth is still an open question. Therefore, the analytical tools to analyze the splitting operators are missing, due to a lack of precise estimates on the exact solution. Typically, all the results presented here highly rely on the fact that a WKB regime is considered.

1.4. **Weakly nonlinear regime.** We now consider the case $\alpha \geqslant 1$ in (1.1), which turns out to be quite easier to treat. To begin with, the assumption on the nonlinearity is weaker, and we allow local interactions.

Assumption 1.8. *The nonlinearity f is of the form $f = f_1 + f_2$, where f_1 satisfies Assumption 1.2, and $f_2 \in C^\infty([0,\infty);\mathbf{R}_+)$, with $f_2(0) = 0$.*

Remark 1.9. The assumption $f_2(0) = 0$ is here merely to simplify the presentation, since replacing f with $f - f_2(0)$ in (1.1) amounts to replacing u^ε with $u^\varepsilon e^{itf_2(0)/\varepsilon}$.

Proposition 1.10. *Suppose that $d \geqslant 1$, f satisfies Assumption 1.8, and that $\alpha \geqslant 1$ in (1.1). Let $(\phi_0, a_0) \in H^{s+2} \times H^s$ with $s > d/2 + 2$. Let $T > 0$ be such that the solution to*

$$\partial_t \phi + \frac{1}{2}|\nabla \phi|^2 = 0; \quad \phi_{|t=0} = \phi_0$$

satisfies $\phi \in C([0,T];H^{s+2})$. Consider $u^\varepsilon = S_\varepsilon^t u_0^\varepsilon$ solution to (1.1) with $\alpha \geqslant 1$ and u_0^ε given by (1.2). There exist $\varepsilon_0 > 0$ and C, c_0 independent of $\varepsilon \in (0,\varepsilon_0]$ such that for all $\Delta t \in (0, c_0]$, for all $n \in \mathbf{N}$ such that $n\Delta t \in [0,T]$, the following holds:
1. *If we set $a^\varepsilon = u^\varepsilon e^{-i\phi/\varepsilon}$, then*

$$\sup_{t\in[0,T]} \|a^\varepsilon(t)\|_{H^s(\mathbf{R}^d)} \leqslant C, \quad \forall \varepsilon \in (0,\varepsilon_0].$$

2. *There exist ϕ_n^ε and a_n^ε with*

$$\|a_n^\varepsilon\|_{H^s(\mathbf{R}^d)} + \|\phi_n^\varepsilon\|_{H^{s+2}(\mathbf{R}^d)} \leqslant C, \quad \forall \varepsilon \in (0,\varepsilon_0],$$

such that $(Z_\varepsilon^{\Delta t})^n \left(a_0 e^{i\phi_0/\varepsilon}\right) = a_n^\varepsilon e^{i\phi_n/\varepsilon}$, and the following error estimate holds:

$$\|a_n^\varepsilon - a^\varepsilon(t_n)\|_{H^{s-2}} + \|\phi_n^\varepsilon - \phi(t_n)\|_{H^s} \leqslant C\Delta t.$$

In particular,

$$\left\|(Z_\varepsilon^{\Delta t})^n u_0^\varepsilon - S_\varepsilon^{n\Delta t} u_0^\varepsilon\right\|_{L^2} \leqslant C\frac{\Delta t}{\varepsilon}.$$

It may seem surprising that even in the weakly nonlinear regime $\alpha = 1$, the result is local in time, and valid only before the possible formation of caustics. As a matter of fact, the behavior of the nonlinear solution u^ε is essentially not understood past the caustic; see e.g. [7].

Notations. Throughout the text, all the constants are independent of $\varepsilon \in (0,1]$. For $(\alpha^\varepsilon)_{0<\varepsilon\leqslant 1}$ and $(\beta^\varepsilon)_{0<\varepsilon\leqslant 1}$ two families of positive real numbers, we write $\alpha^\varepsilon \lesssim \beta^\varepsilon$ if $\limsup_{\varepsilon\to 0} \alpha^\varepsilon/\beta^\varepsilon < \infty$.

2. Action of the numerical scheme in the WKB regime

Our approach consists in sticking to the WKB framework. We write the solutions to (1.1), under the form

$$a^\varepsilon(t,x)e^{i\phi^\varepsilon(t,x)/\varepsilon}, \tag{2.1}$$

with a^ε and ϕ^ε bounded in $H^s(\mathbf{R}^d)$ *uniformly in* $\varepsilon \in (0,1]$. Here, the "phase" ϕ^ε is real-valued, and the "amplitude" a^ε is complex-valued; of course, such a representation is not unique. As a matter of fact, both a^ε and ϕ^ε must be expected to depend on ε. Functions of this form will be referred to as *WKB states* throughout the text. From now on, and up to Section 7, we assume $\alpha = 0$ in (1.1).

2.1. **A stable phase/amplitude decomposition.** The important remark consists in noticing that the flows associated to (1.5) and (1.6) preserve the structure of WKB states.

Nonlinear flow. In the case of the nonlinear flow (1.6), the exact formula (1.7) shows immediately that a WKB state evolves as a WKB state: if $w^\varepsilon_{|t=0} = \alpha^\varepsilon e^{i\varphi^\varepsilon/\varepsilon}$, then the solution to (1.6) is given by

$$w^\varepsilon(t,x) = \alpha^\varepsilon(x) e^{i\left(\varphi^\varepsilon(x) - tf\left(|\alpha^\varepsilon(x)|^2\right)\right)/\varepsilon}.$$

This is indeed of the form (2.1), with

$$a^\varepsilon(t,x) = \alpha^\varepsilon(x), \quad \phi^\varepsilon(t,x) = \varphi^\varepsilon(x) - tf\left(|\alpha^\varepsilon(x)|^2\right).$$

We can therefore rewrite the action of Y^t_ε on WKB states as the action of the flow $\mathcal{Y}^\varepsilon_t$ on phase/amplitude pairs (ϕ, a) characterized by

$$\begin{cases} \partial_t \phi^\varepsilon + f\left(|a^\varepsilon|^2\right) = 0; \quad \phi^\varepsilon_{|t=0} = \phi^\varepsilon_0, \\ \partial_t a^\varepsilon = 0; \quad a^\varepsilon_{|t=0} = a^\varepsilon_0. \end{cases} \tag{2.2}$$

Linear flow. The analysis of the linear flow (1.4) is less straightforward, and requires more care than the nonlinear flow. Consider the system

$$\begin{cases} \partial_t \phi^\varepsilon + \dfrac{1}{2}|\nabla \phi^\varepsilon|^2 = 0; \quad \phi^\varepsilon_{|t=0} = \phi^\varepsilon_0, \\ \partial_t a^\varepsilon + \nabla\phi^\varepsilon \cdot \nabla a^\varepsilon + \dfrac{1}{2} a^\varepsilon \Delta \phi^\varepsilon = i\dfrac{\varepsilon}{2}\Delta a^\varepsilon; \quad a^\varepsilon_{|t=0} = a^\varepsilon_0. \end{cases} \tag{2.3}$$

Note that this is not exactly the system corresponding to standard WKB analysis, because of the term $\varepsilon \Delta a^\varepsilon$ in the second equation, which is discarded in WKB approximation. The first equation is an eikonal equation, which has a smooth solution at least locally in time (see e.g. [7]), and energy estimates then follow easily for the second equation. We emphasize the fact that (2.3) is *equivalent* to (1.4) in the case of initial WKB states (2.1), at least locally in time, *modulo* the eikonal equation. Indeed, given an initial phase ϕ^ε_0, we can solve, locally in time, the eikonal equation

$$\partial_t \phi^\varepsilon + \frac{1}{2}|\nabla\phi^\varepsilon|^2 = 0; \quad \phi^\varepsilon_{|t=0} = \phi^\varepsilon_0. \tag{2.4}$$

In general, the solution to (2.4) does not remain smooth for all time, due to the formation of caustics (see e.g. [7]). We note that $w^\varepsilon = \nabla \phi^\varepsilon$ solves a (multidimensional) Burgers equation

$$\partial_t w^\varepsilon + w^\varepsilon \cdot \nabla w^\varepsilon = 0; \quad w^\varepsilon_{|t=0} = \nabla \phi^\varepsilon_0.$$

This remark will be used to derive *a priori* estimates for the system (2.3). Once ϕ^ε is known, then v^ε, solution to (1.4), and a^ε, are related through the formula

$$v^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon},$$

which yields an obvious bijective correspondence between these two functions (for a fixed ϕ^ε). Even though there is no uniqueness in the choice of ϕ^ε, we conclude that if the initial datum is a WKB state, $v^\varepsilon_{|t=0} = a^\varepsilon_0 e^{i\phi^\varepsilon_0/\varepsilon}$, then at least locally in time, v^ε remains a WKB state, since it can be written as $v^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$, where $(\phi^\varepsilon, a^\varepsilon)$ is the solution to (2.3). Following the same convention as in the case of the nonlinear flow, we denote by $\mathcal{X}_\varepsilon^t$ the flow acting of phase/amplitude pairs,

$$\mathcal{X}_\varepsilon^t \begin{pmatrix} \phi_0^\varepsilon \\ a_0^\varepsilon \end{pmatrix} = \begin{pmatrix} \phi^\varepsilon(t) \\ a^\varepsilon(t) \end{pmatrix},$$

where $(\phi^\varepsilon, a^\varepsilon)$ is the solution to (2.3). Similary, we write $\mathcal{Z}_\varepsilon^t = \mathcal{Y}_\varepsilon^t \mathcal{X}_\varepsilon^t$.

2.2. **Rewriting the splitting method in the WKB regime.** Instead of analyzing directly the equations (1.4)–(1.6), we shall work on (2.3)–(2.2), in view of the previous subsection. We denote by Π^ε the wave reconstruction operator

$$\Pi^\varepsilon \begin{pmatrix} \phi^\varepsilon \\ a^\varepsilon \end{pmatrix} = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon},$$

and we note the identity, which is the key conclusion of the above analysis:

$$\Pi^\varepsilon \mathcal{Z}_t^\varepsilon \begin{pmatrix} \phi^\varepsilon \\ a^\varepsilon \end{pmatrix} = Z_t^\varepsilon \left(a^\varepsilon e^{i\phi^\varepsilon/\varepsilon} \right). \tag{2.5}$$

In view of the obvious remark

$$\Pi^\varepsilon \begin{pmatrix} \phi \\ a \end{pmatrix} = \Pi^\varepsilon \begin{pmatrix} \phi - \varepsilon\theta \\ a e^{i\theta} \end{pmatrix}, \quad \forall \theta \in \mathbf{R},$$

we see that working with $(\phi^\varepsilon, a^\varepsilon)$ is not equivalent to working with the wave function $a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$. However, we only use the fact that the numerical solution can be represented by this decomposition, and no uniqueness argument is needed, except the fact that the solutions to (1.4) and (1.6), respectively, are unique.

We finally notice that the form (2.1) (with a^ε and ϕ^ε bounded in $H^s(\mathbf{R}^d)$ uniformly in ε) is preserved by the exact flow. This is so thanks to the gauge invariance of the nonlinearity, which rules out the appearance of new phases or new harmonics by nonlinear interaction (an aspect which also appears when solving (1.6)). In the case of a local defocusing nonlinearity (typically $f(\rho) = \rho$), recall the original idea of Grenier [16] to study the semi-classical limit for (1.1): seek the solution u^ε to (1.1) under the form (2.1), with ϕ^ε real-valued and a^ε complex-valued. One gains a degree of freedom, and the choice of Grenier consists in imposing

$$\begin{cases} \partial_t \phi^\varepsilon + \frac{1}{2}|\nabla\phi^\varepsilon|^2 + f\left(|a^\varepsilon|^2\right) = 0; \quad \phi^\varepsilon_{|t=0} = \phi_0, \\ \partial_t a^\varepsilon + \nabla\phi^\varepsilon \cdot \nabla a^\varepsilon + \frac{1}{2} a^\varepsilon \Delta\phi^\varepsilon = i\frac{\varepsilon}{2}\Delta a^\varepsilon; \quad a^\varepsilon_{|t=0} = a_0. \end{cases} \tag{2.6}$$

This choice differs from the standard Madelung transform, which is limited by the presence of vacuum (zeroes of a^ε; see [8]). Also, an important technical feature of (2.6) is that the term $i\Delta a^\varepsilon$ is skew-symmetric. Therefore, it plays no role in H^s-energy estimates. In particular, it causes no loss of regularity. Under Assumption 1.2, the adaptation of the approach of Grenier can be found in [1, 20] (see also [21, 24, 25] for the case of Schrödinger-Poisson system in low dimensions, where low frequencies cause technical difficulties). We denote by $\mathcal{S}_t^\varepsilon$ the flow associated to (2.6).

Remark 2.1. In (2.6), the initial data are supposed implicitly independent of ε. This is merely for the sake of consistency in future references. Throughout this paper, the flow associated to (2.6) will be considered for initial data which may depend on ε, but which are uniformly bounded in suitable Sobolev spaces.

Instead of analyzing directly the splitting method for (1.1) as presented in Section 1.1, we shall therefore analyze a splitting method for (2.6): when the term f is discarded, we recover (2.3), which is solved alternatingly with (2.2). The latter system consists indeed in dropping out the Laplacian in (2.6), since all spatial derivatives have disappeared.

3. TECHNICAL BACKGROUND

As noticed in [1], the following lemma turns out to be very helpful.

Lemma 3.1. *Let $s \geqslant 0$. Under Assumption 1.2, there exists C such that*

$$\|\nabla f(\rho)\|_{H^{s+1}(\mathbf{R}^d)} \leqslant C\left(\|\rho\|_{H^s(\mathbf{R}^d)} + \|\rho\|_{L^1(\mathbf{R}^d)}\right), \quad \forall \rho \in H^s(\mathbf{R}^d) \cap L^1(\mathbf{R}^d). \tag{3.1}$$

If in addition $s > d/2$, there exists C such that

$$\|f(\rho)\|_{L^\infty(\mathbf{R}^d)} \leqslant C\left(\|\rho\|_{H^s(\mathbf{R}^d)} + \|\rho\|_{L^1(\mathbf{R}^d)}\right), \quad \forall \rho \in H^s(\mathbf{R}^d) \cap L^1(\mathbf{R}^d). \tag{3.2}$$

Proof. By Plancherel formula,

$$\begin{aligned}\|\nabla f(\rho)\|^2_{H^{s+1}(\mathbf{R}^d)} &= \int_{\mathbf{R}^d} |\xi|^2 \left(1+|\xi|^2\right)^{s+1} |\widehat{K}(\xi)|^2 |\widehat{\rho}(\xi)|^2 d\xi \\ &\leqslant \left(\sup_{\xi \in \mathbf{R}^d} \left(1+|\xi|^2\right)|\widehat{K}(\xi)|\right)^2 \|\rho\|^2_{H^s},\end{aligned}$$

hence (a weaker version of) the lemma in the first case of Assumption 1.2. If $d \geqslant 3$,

$$\begin{aligned}\int_{|\xi|\leqslant 1} |\xi|^2 \left(1+|\xi|^2\right)^{s+1} |\widehat{K}(\xi)|^2 |\widehat{\rho}(\xi)|^2 d\xi &\leqslant \left(\sup_{\xi\in\mathbf{R}^d} |\xi|^2 |\widehat{K}(\xi)|\right)^2 \int_{|\xi|\leqslant 1} |\xi|^{-2} |\widehat{\rho}(\xi)|^2 d\xi \\ &\leqslant C\|\widehat{\rho}\|^2_{L^\infty(\mathbf{R}^d)} \int_0^1 r^{d-3} dr \leqslant C\|\rho\|^2_{L^1(\mathbf{R}^d)},\end{aligned}$$

where we have used spherical coordinates and Hausdorff-Young's inequality. This yields the first part of the lemma. For the second part, we use the same tools,

$$\|f(\rho)\|_{L^\infty} \leqslant (2\pi)^{-d/2} \|\widehat{f(\rho)}\|_{L^1} = \|\widehat{K}\widehat{\rho}\|_{L^1}.$$

Split the integral between the two regions $\{|\xi| \leqslant 1\}$ and $\{|\xi| > 1\}$:

$$\begin{aligned}&\int_{|\xi|\leqslant 1} |\widehat{K}(\xi)||\widehat{\rho}(\xi)| d\xi \leqslant C\|\widehat{\rho}\|_{L^\infty} \int_0^1 r^{d-1} \left|\widehat{K}(r)\right| dr \lesssim \|\rho\|_{L^1}, \\ &\int_{|\xi|>1} |\widehat{K}(\xi)||\widehat{\rho}(\xi)| d\xi \leqslant C\|\widehat{\rho}\|_{L^1} \lesssim \|\rho\|_{H^s}, \quad \text{since } s > d/2.\end{aligned}$$

This estimate is not sharp, since we do not use the decay of $\widehat{K}$ at infinity. □

As in [1], we infer the following result, concerning the exact solution, that is, the solution to (2.6). This result implies the first point of Theorem 1.5.

Proposition 3.2. *Suppose that $d \geqslant 1$, and that f satisfies Assumption 1.2. Let $(\nabla\phi_0, a_0) \in H^{s+1} \times H^s$ with $s > d/2 + 1$, and let $T > 0$ be such that the solution to (1.12) satisfies $(v, \rho) \in C([0,T]; H^{s+1} \times H^s)$. Then there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0]$, (2.6) has a unique solution, which satisfies $(\nabla\phi^\varepsilon, a^\varepsilon) \in$*

$C([0,T];H^{s+1}\times H^s)$, uniformly in $\varepsilon\in(0,\varepsilon_0]$: there exists $C(T,\|a_0\|_{H^s},\|\nabla\phi_0\|_{H^{s+1}})$ independent of $\varepsilon\in(0,\varepsilon_0]$ such that

$$\sup_{t\in[0,T]}\left(\|a^\varepsilon(t)\|_{H^s(\mathbf{R}^d)}+\|\nabla\phi^\varepsilon(t)\|_{H^{s+1}(\mathbf{R}^d)}\right)\leqslant C\left(T,\|a_0\|_{H^s(\mathbf{R}^d)},\|\nabla\phi_0\|_{H^{s+1}(\mathbf{R}^d)}\right).$$

If in addition $\phi_0\in L^\infty(\mathbf{R}^d)$, then $\phi^\varepsilon\in C([0,T];L^\infty(\mathbf{R}^d))$ and

$$\sup_{t\in[0,T]}\|\phi^\varepsilon(t)\|_{L^\infty(\mathbf{R}^d)}\leqslant\|\phi_0\|_{L^\infty}+\underline{C}\left(T,\|a_0\|_{H^s(\mathbf{R}^d)},\|\nabla\phi_0\|_{H^{s+1}(\mathbf{R}^d)}\right).$$

Sketch of the proof. Let $w^\varepsilon=\nabla\phi^\varepsilon$. By differentiating in space the first equation in (2.6), we see that any solution to (2.6) must solve

$$\begin{cases}\partial_t w^\varepsilon+w^\varepsilon\cdot\nabla w^\varepsilon+\nabla f\left(|a^\varepsilon|^2\right)=0; & w^\varepsilon_{|t=0}=\nabla\phi_0,\\ \partial_t a^\varepsilon+w^\varepsilon\cdot\nabla a^\varepsilon+\dfrac{1}{2}a^\varepsilon\operatorname{div}w^\varepsilon=i\dfrac{\varepsilon}{2}\Delta a^\varepsilon; & a^\varepsilon_{|t=0}=a_0.\end{cases}\tag{3.3}$$

The left hand side corresponds to a hyperbolic symmetric system for the unknown $(w^\varepsilon,\operatorname{Re}a^\varepsilon,\operatorname{Im}a^\varepsilon)\in\mathbf{R}^{d+2}$, thanks to Lemma 3.1, and the shift in regularity between $w^\varepsilon\in H^{s+1}$ and $a^\varepsilon\in H^s$. The right hand side of (3.3) is a skew-symmetric term, which does not appear in H^s energy estimates. The key point to notice is that unlike what would happen in the case of the nonlinear Schrödinger equation, the terms $\nabla f(|a^\varepsilon|^2)$ and $a^\varepsilon\operatorname{div}w^\varepsilon$ are not quasilinear, but semilinear (they can be treated as perturbations), in view of Lemma 3.1 and the functional framework. By standard theory (see e.g. [2]), (3.3) has a unique solution $(w^\varepsilon,a^\varepsilon)\in C([0,\tau];H^{s+1}\times H^s)$, for some $\tau>0$ independent of $\varepsilon\in(0,1]$.

We can take $\tau\geqslant T$ for ε sufficiently small. Indeed, if T' denotes the lifespan of (3.3) in the case $\varepsilon=0$, then necessarily $T'>T$, for if we had $T'\leqslant T$, then by uniqueness for the Euler-Poisson system, $|a|^2=\rho\in C([0,T];H^s\cap L^1)$ and $w=v\in C([0,T];H^{s+1})$. Back to the transport equation in (3.3), we infer that $a\in L^\infty([0,T];H^s)$, which yields a contradiction.

Finally, we note that a^ε, w^ε and ϕ^ε are related through the formula

$$\partial_t\phi^\varepsilon+\frac{1}{2}|w^\varepsilon|^2+f\left(|a^\varepsilon|^2\right)=0;\quad \phi^\varepsilon_{|t=0}=\phi_0$$

Therefore, if w^ε and a^ε are known, then ϕ^ε is obtained by a simple integration in time, and the last estimate of the proposition follows from (3.2). □

Note that the above result is expected to be valid only locally in time, since the solution to (1.12) may develop a singularity in finite time. In that case for fixed $\varepsilon>0$, a^ε may become singular, or remain smooth but become ε-oscillatory for large time, as suggested by the simulations in [9]. This can be understood as follows: for large time, several oscillations are expected in u^ε, so they cannot be carried by only one exponential function as in (2.1), therefore, a^ε becomes rapidly oscillatory, and its H^s-norm is not bounded uniformly in $\varepsilon\in(0,1]$.

The analysis of [1] also implies the following result.

Proposition 3.3. *Let $d\geqslant 1$, and f satisfying Assumption 1.8. Let $R>0$ and $s>d/2+2$. There exists $T=T(R)>0$ such that if*

$$\|a_0\|_{H^s(\mathbf{R}^d)}+\|\nabla\phi_0\|_{H^{s+1}(\mathbf{R}^d)}\leqslant R,$$

then (1.12) *has a unique solution* $(v,\rho)\in C([0,T];H^{s+1}\times H^s)$. *There exist* $\varepsilon_0>0$ *and* $K=K(R)$ *independent of* $\varepsilon\in(0,\varepsilon_0]$ *such that if in addition* $(\nabla\varphi_0,b_0)\in H^{s+1}\times H^s$ *satisfies*

$$\|b_0\|_{H^s(\mathbf{R}^d)}+\|\nabla\varphi_0\|_{H^{s+1}(\mathbf{R}^d)}\leqslant R,$$

then for all $t\in[0,T]$, *the solutions to* (2.6) *with initial data* (ϕ_0,a_0) *and* (φ_0,b_0), *respectively, satisfy:*

$$\|a^\varepsilon(t)-b^\varepsilon(t)\|_{H^s}+\|\nabla\phi^\varepsilon(t)-\nabla\varphi^\varepsilon(t)\|_{H^{s+1}}\leqslant K\left(\|a_0-b_0\|_{H^s}+\|\nabla\phi_0-\nabla\varphi_0\|_{H^{s+1}}\right).$$

There exists $\kappa=\kappa(R)$ *such that if in addition* $\phi_0,\varphi_0\in L^\infty(\mathbf{R}^d)$, *then*

$$\|\phi^\varepsilon(t)-\varphi^\varepsilon(t)\|_{L^\infty}\leqslant\|\phi_0-\varphi_0\|_{L^\infty}+\kappa\left(\|a_0-b_0\|_{H^s}+\|\nabla\phi_0-\nabla\varphi_0\|_{H^{s+1}}\right).$$

4. Estimating the approximate flow

In this section, we prove various estimates concerning the flows involved in the definition of the numerical scheme, $\mathcal{X}_\varepsilon^t$ and $\mathcal{Y}_\varepsilon^t$.

4.1. **The nonlinear operator.**

Unlike what happens in most cases when studying splitting operators, the most delicate operator to control is the linear one, denoted here by $\mathcal{X}_\varepsilon^t$, while in the present framework, $\mathcal{Y}_\varepsilon^t$ turns out to be the simpler of the two.

Lemma 4.1. *Let* $s>d/2$ *and* $\phi_0^\varepsilon,a_0^\varepsilon\in\mathcal{S}'(\mathbf{R}^d)$, *with* $(\nabla\phi_0^\varepsilon,a_0^\varepsilon)\in H^{s+1}\times H^s$, *for some* $s>d/2$. *The solution to* (2.2) *is given by*

$$\phi^\varepsilon(t)=\phi_0^\varepsilon-tf\left(|a_0^\varepsilon|^2\right);\quad a^\varepsilon(t)=a_0^\varepsilon.$$

In particular, there exists $C=C(\mu)$ *such that if* $\|a_0^\varepsilon\|_{L^\infty}\leqslant\mu$,

$$\|a^\varepsilon(t)\|_{H^s}=\|a_0^\varepsilon\|_{H^s},\quad\|\nabla\phi^\varepsilon(t)\|_{H^{s+1}}\leqslant\|\nabla\phi_0^\varepsilon\|_{H^{s+1}}+Ct\|a_0^\varepsilon\|_{H^s},\quad\forall t\geqslant 0.$$

Finally, if $\phi_0^\varepsilon\in L^\infty(\mathbf{R}^d)$, *then there exists* $C=C(\mu)$ *such that if* $\|a_0^\varepsilon\|_{L^\infty}\leqslant\mu$,

$$\|\phi^\varepsilon(t)\|_{L^\infty}\leqslant\|\phi_0^\varepsilon\|_{L^\infty}+Ct\|a_0^\varepsilon\|_{H^s},\quad\forall t\geqslant 0.$$

Proof. Since $s>d/2$, $H^s(\mathbf{R}^d)$ is a Banach algebra embedded into $C(\mathbf{R}^d)$, hence the formula for ϕ^ε. The estimates are straightforward consequences of Lemma 3.1, and of the tame estimate $\|fg\|_{H^s}\lesssim\|f\|_{L^\infty}\|g\|_{H^s}+\|f\|_{H^s}\|g\|_{L^\infty}$. □

4.2. **The linear operator.**

We now consider (2.3). The following lemma is a variant of [17, Lemma 3.2]. Like in that paper, the key aspect of the result is the at-most-geometric-growth of $\mathbf{v}$, which will be crucial in the context of the splitting approach, where this control will be used on a time step.

Lemma 4.2. *Let* $s>d/2+1$ *and* $\mu>0$. *There exists* $\tau=\tau(\mu)>0$ *such that if*

$$\|\mathbf{v}_0\|_{H^s}\leqslant\mu,$$

then the (multi-dimensional) Burgers equation

$$\partial_t\mathbf{v}+\mathbf{v}\cdot\nabla\mathbf{v}=0;\quad\mathbf{v}_{|t=0}=\mathbf{v}_0\tag{4.1}$$

has a unique solution $\mathbf{v}\in C([0,\tau];H^s)$, *which satisfies*

$$\sup_{t\in[0,\tau]}\|\mathbf{v}(t)\|_{H^s}\leqslant 2\mu.$$

Proof. Local existence of a unique H^s solution follows from a global inversion theorem (see e.g. [7]), so we focus on the energy estimate. We have

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{v}\|_{H^s}^2 = \langle \mathbf{v}, \partial_t \mathbf{v}\rangle_{H^s} = \langle \Lambda^s \mathbf{v}, \Lambda^s \partial_t \mathbf{v}\rangle_{L^2} = -\left\langle \Lambda^s \mathbf{v}, \Lambda^s \left(\mathbf{v}\cdot\nabla\mathbf{v}\right)\right\rangle_{L^2},$$

where $\Lambda = (1-\Delta)^{1/2}$. Introduce the commutator

$$\frac{1}{2}\frac{d}{dt}\|\mathbf{v}\|_{H^s}^2 = -\left\langle \Lambda^s \mathbf{v}, \mathbf{v}\cdot\nabla\Lambda^s\mathbf{v}\right\rangle_{L^2} + \left\langle \Lambda^s \mathbf{v}, \mathbf{v}\cdot\nabla\Lambda^s\mathbf{v} - \Lambda^s\left(\mathbf{v}\cdot\nabla\mathbf{v}\right)\right\rangle_{L^2}.$$

By integration by parts, the first term is controlled by

$$\left|\left\langle \Lambda^s \mathbf{v}, \mathbf{v}\cdot\nabla\Lambda^s\mathbf{v}\right\rangle_{L^2}\right| \leqslant \frac{1}{2}\|\mathbf{v}\|_{H^s}^2\|\operatorname{div}\mathbf{v}\|_{L^\infty} \lesssim \|\mathbf{v}\|_{H^s}^3,$$

where we have used Sobolev embedding and the assumption $s > d/2+1$. The last term is estimated thanks to Kato-Ponce estimate [19]

$$\|\Lambda^s(fg) - f\Lambda^s g\|_{L^2} \lesssim \|\nabla f\|_{L^\infty}\|g\|_{H^{s-1}} + \|f\|_{H^s}\|g\|_{L^\infty}, \tag{4.2}$$

with $f = \mathbf{v}$ and $g = \nabla\mathbf{v}$:

$$\begin{aligned}\left|\left\langle \Lambda^s \mathbf{v}, \mathbf{v}\cdot\nabla\Lambda^s\mathbf{v} - \Lambda^s\left(\mathbf{v}\cdot\nabla\mathbf{v}\right)\right\rangle_{L^2}\right| &\leqslant \|\mathbf{v}\|_{H^s}\left\|\Lambda^s\left(\mathbf{v}\cdot\nabla\mathbf{v}\right) - \mathbf{v}\cdot\nabla\Lambda^s\mathbf{v}\right\|_{L^2}\\ &\lesssim \|\nabla\mathbf{v}\|_{L^\infty}\|\mathbf{v}\|_{H^s}^2 \lesssim \|\mathbf{v}\|_{H^s}^3.\end{aligned}$$

We infer $\frac{d}{dt}\|\mathbf{v}\|_{H^s} \leqslant C\|\mathbf{v}\|_{H^s}^2$, and the result follows by comparing with the ordinary differential equation $\dot{y} = Cy^2$. □

Lemma 4.3. *Let $s > d/2+1$ and $\mu > 0$. If the solution $\mathbf{v}$ to (4.1) satisfies*

$$\|\nabla\mathbf{v}(t)\|_{L^\infty} \leqslant \mu, \quad 0 \leqslant t \leqslant \tau,$$

then there exists c independent of μ and τ such that

$$\sup_{t\in[0,\tau]}\|\mathbf{v}(t)\|_{H^s} \leqslant e^{c\mu t}\|\mathbf{v}(0)\|_{H^s}, \quad 0 \leqslant t \leqslant \tau.$$

Proof. This lemma is a straightforward consequence of the tame estimates used in the proof of Lemma 4.2. □

Proposition 4.4. *Let $\sigma > d/2$, $\mu > 0$. Suppose that $(\nabla\phi_0^\varepsilon, a_0^\varepsilon) \in H^{\sigma+1}\times H^\sigma$, with*

$$\|\nabla\phi_0^\varepsilon\|_{H^{\sigma+1}} \leqslant \mu, \quad \|a_0^\varepsilon\|_{H^\sigma} \leqslant \mu.$$

There exists $\tau = \tau(\mu)$ independent of ε such that (2.3) has a unique solution, with $(\nabla\phi^\varepsilon, a^\varepsilon) \in C([0,\tau]; H^{\sigma+1}\times H^\sigma)$, and

$$\sup_{t\in[0,\tau]}\|\nabla\phi^\varepsilon(t)\|_{H^{\sigma+1}} \leqslant 2\mu, \quad \sup_{t\in[0,\tau]}\|a^\varepsilon(t)\|_{H^\sigma} \leqslant 2\mu.$$

If in addition $\phi_0^\varepsilon \in L^\infty(\mathbf{R}^d)$, then $\phi^\varepsilon \in C([0,\tau]; L^\infty)$ and

$$\sup_{t\in[0,\tau]}\|\phi^\varepsilon(t)\|_{L^\infty} \leqslant \|\phi_0^\varepsilon\|_{L^\infty} + \tau\mu.$$

Proof. From Lemma 4.2, (4.1) has a unique solution $\mathbf{v} \in C([0,\tau]; H^{\sigma+1})$, such that $\mathbf{v}_{|t=0} = \nabla\phi_0^\varepsilon$, with $\|\mathbf{v}(t)\|_{H^{\sigma+1}} \leqslant 2\mu$ for $t \in [0,\tau]$. Now let

$$\phi^\varepsilon(t) = \phi_0^\varepsilon - \frac{1}{2}\int_0^t |\mathbf{v}(\sigma)|^2 d\sigma.$$

We note that $\partial_t(\mathbf{v} - \nabla\phi^\varepsilon) = \partial_t\mathbf{v} - \nabla\partial_t\phi^\varepsilon = 0$, so $\mathbf{v} = \nabla\phi^\varepsilon$, and the result concerning ϕ^ε follows.

The existence of a solution a^ε follows for instance from the fact that it is given by $a^\varepsilon = v^\varepsilon e^{-i\phi^\varepsilon/\varepsilon}$, where $v^\varepsilon \in C(\mathbf{R}; H^\sigma)$ is the solution to the linear Schrödinger equation (1.4) with initial datum $a_0^\varepsilon e^{i\phi_0^\varepsilon/\varepsilon} \in H^\sigma$. So we are left with the energy estimate: since $i\Delta$ is skew-symmetric,

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|a^\varepsilon\|_{H^\sigma}^2 &= \left\langle \Lambda^\sigma a^\varepsilon, \left(\partial_t - i\frac{\varepsilon}{2}\Delta\right)\Lambda^\sigma a^\varepsilon\right\rangle_{L^2}\\ &= -\left\langle \Lambda^\sigma a^\varepsilon, \Lambda^\sigma\left(\nabla\phi^\varepsilon\cdot\nabla a^\varepsilon + \frac{1}{2}a^\varepsilon\Delta\phi^\varepsilon\right)\right\rangle_{L^2}.\end{aligned}$$

By integration by parts,

$$\left\langle \Lambda^\sigma a^\varepsilon, \nabla\phi^\varepsilon\cdot\nabla\Lambda^\sigma a^\varepsilon + \frac{1}{2}\Lambda^\sigma a^\varepsilon\Delta\phi^\varepsilon\right\rangle_{L^2} = 0,$$

so we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|a^\varepsilon\|_{H^\sigma}^2 &= \left\langle \Lambda^\sigma a^\varepsilon, \nabla\phi^\varepsilon\cdot\nabla\Lambda^\sigma a^\varepsilon - \Lambda^\sigma\left(\nabla\phi^\varepsilon\cdot\nabla a^\varepsilon\right)\right\rangle_{L^2}\\ &\quad + \frac{1}{2}\left\langle \Lambda^\sigma a^\varepsilon, \Lambda^\sigma a^\varepsilon\Delta\phi^\varepsilon - \Lambda^\sigma\left(a^\varepsilon\Delta\phi^\varepsilon\right)\right\rangle_{L^2}.\end{aligned}$$

Kato-Ponce estimate (4.2) for the first line, and tame estimates for the second line then yield

$$\begin{aligned}\frac{d}{dt}\|a^\varepsilon\|_{H^\sigma}^2 &\lesssim \|a^\varepsilon\|_{H^\sigma}\Big(\|a^\varepsilon\|_{H^\sigma}\|\nabla^2\phi^\varepsilon\|_{L^\infty} + \|\nabla\phi^\varepsilon\|_{H^\sigma}\|\nabla a\|_{L^\infty}\\ &\qquad + \|\Delta\phi^\varepsilon\|_{L^\infty}\|a^\varepsilon\|_{H^\sigma} + \|\Delta\phi^\varepsilon\|_{H^\sigma}\|a\|_{L^\infty}\Big)\\ &\lesssim \|\nabla\phi^\varepsilon\|_{H^{\sigma+1}}\|a^\varepsilon\|_{H^\sigma}^2,\end{aligned}\tag{4.3}$$

since $\sigma > d/2$, and the result follows from Gronwall lemma, by decreasing τ if necessary. □

Remark 4.5. The above proof suggests that the shift in regularity, between ϕ^ε and a^ε, cannot be avoided. Note that this phenomenon shows up when the *free* Schrödinger equation (1.4) is solved, in terms of WKB states, and is not a difficulty due to the nonlinear aspect of (1.1).

Proposition 4.6. *Let $\sigma > d/2$, $\mu > 0$. Suppose that the solution to* (2.3) *satisfies*

$$\|\nabla\phi^\varepsilon(t)\|_{W^{1,\infty}} \leqslant \mu, \quad \|a^\varepsilon(t)\|_{W^{1,\infty}} \leqslant \mu, \quad 0 \leqslant t \leqslant \tau.$$

There exists c independent of ε, μ, τ such that the solution to (2.3) *satisfies*

$$\|\nabla\phi^\varepsilon(t)\|_{H^{\sigma+1}} + \|a^\varepsilon(t)\|_{H^\sigma} \leqslant e^{c\mu t}\left(\|\nabla\phi_0^\varepsilon\|_{H^{\sigma+1}} + \|a_0^\varepsilon\|_{H^\sigma}\right), \quad 0 \leqslant t \leqslant \tau.$$

Proof. Lemma 4.3 readily implies

$$\|\nabla\phi^\varepsilon(t)\|_{H^{\sigma+1}} \leqslant e^{c\mu t}\|\nabla\phi_0^\varepsilon\|_{H^{\sigma+1}}, \quad 0 \leqslant t \leqslant \tau,$$

for some c independent of ε, μ, τ. Back to the proof of Proposition 4.4, simply apply Gronwall lemma to (4.3). □

4.3. **The splitting operator.** In view of Lemma 4.1 and Proposition 4.4, we readily have:

Corollary 4.7. *Let $s > d/2$, $\mu > 0$. Suppose that $(\nabla\phi_0^\varepsilon, a^\varepsilon) \in H^{s+1} \times H^s$, with*

$$\|\nabla\phi_0^\varepsilon\|_{H^{s+1}} \leqslant \mu, \quad \|a_0^\varepsilon\|_{H^s} \leqslant \mu.$$

There exists $\tau = \tau(\mu) > 0$ independent of ε such that $\mathcal{Z}_\varepsilon^t \begin{pmatrix} \phi_0^\varepsilon \\ a_0^\varepsilon \end{pmatrix} = \begin{pmatrix} \phi_t^\varepsilon \\ a_t^\varepsilon \end{pmatrix}$, with

$$\sup_{t\in[0,\tau]} \|\nabla\phi_t^\varepsilon\|_{H^{s+1}} \leqslant 4\mu, \quad \sup_{t\in[0,\tau]} \|a_t^\varepsilon\|_{H^s} \leqslant 4\mu.$$

If in addition $\phi_0^\varepsilon \in L^\infty$, with $\|\phi_0^\varepsilon\|_{L^\infty} \leqslant \mu$, then, up to decreasing τ, we have

$$\sup_{t\in[0,\tau]} \|\phi_t^\varepsilon\|_{L^\infty} \leqslant 4\mu.$$

Proof. Lemma 4.1 implies that $\mathcal{Y}_\varepsilon^t \begin{pmatrix} \phi_0^\varepsilon \\ a_0^\varepsilon \end{pmatrix} = \begin{pmatrix} \varphi_t^\varepsilon \\ \alpha_t^\varepsilon \end{pmatrix}$, with

$$\|\alpha_t^\varepsilon\|_{H^s} = \|a_0^\varepsilon\|_{H^s}, \quad \|\nabla\varphi_t^\varepsilon\|_{H^{s+1}} \leqslant \mu + Ct, \quad t \geqslant 0.$$

We then apply Proposition 4.4 with $\sigma = s$. We note that the L^∞ regularity for the phase is propagated by both operators, and the estimate follows easily. □

In view of Lemma 4.1 and Proposition 4.6, we also infer:

Corollary 4.8. *Let $s > d/2$, $\mu > 0$. Suppose that $\mathcal{Z}_\varepsilon^t \begin{pmatrix} \phi_0^\varepsilon \\ a_0^\varepsilon \end{pmatrix} = \begin{pmatrix} \phi_t^\varepsilon \\ a_t^\varepsilon \end{pmatrix}$, with*

$$\|\nabla\phi_t^\varepsilon\|_{W^{1,\infty}} \leqslant \mu, \quad \|a_t^\varepsilon\|_{W^{1,\infty}} \leqslant \mu, \quad 0 \leqslant t \leqslant \tau.$$

Then there exists c independent of ε, μ, τ, such that

$$\|\nabla\phi_t^\varepsilon\|_{H^{s+1}} + \|a_t^\varepsilon\|_{H^s} \leqslant e^{c\mu t}\left(\|\nabla\phi_0^\varepsilon\|_{H^{s+1}} + \|a_0^\varepsilon\|_{H^s}\right), \quad 0 \leqslant t \leqslant \tau.$$

5. LOCAL ERROR ESTIMATE

We recall the result (and resume the notations) from [13] concerning the local error estimate in the context of (1.1). For a possibly nonlinear operator A, we denote by $\mathcal{E}_A$ the associated flow:

$$\partial_t \mathcal{E}_A(t,v) = A\left(\mathcal{E}_A(t,v)\right); \quad \mathcal{E}_A(0,v) = v.$$

The results presented in this section rely heavily on the following result.

Theorem 5.1 (Theorem 1 from [13])**.** *Suppose that $F(u) = A(u) + B(u)$, and denote by*

$$\mathcal{S}^t(u) = \mathcal{E}_F\left(t,u\right) \text{ and } \mathcal{Z}^t(u) = \mathcal{E}_B\left(t, \mathcal{E}_A(t,u)\right)$$

the exact flow and the Lie-Trotter flow, respectively. Let $\mathcal{L}(t,u) = \mathcal{Z}^t(u) - \mathcal{S}^t(u)$. We have the exact formula

$$\mathcal{L}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2\mathcal{E}_F\left(t-\tau_1, \mathcal{Z}^{\tau_1}(u)\right) \partial_2\mathcal{E}_B\left(\tau_1-\tau_2, \mathcal{E}_A(\tau_1,u)\right) \times [B,A]\left(\mathcal{E}_B\left(\tau_2, \mathcal{E}_A\left(\tau_1,u\right)\right)\right) d\tau_2 d\tau_1.$$

We emphasize the fact that in [13], this result is established for general operators A and B. In particular, both operators may be nonlinear. In the case of (1.4)–(1.6),

$$A = i\frac{\varepsilon}{2}\Delta; \quad B(v) = -\frac{i}{\varepsilon}f\left(|v|^2\right)v; \quad F(v) = A(v) + B(v).$$

We have omitted the dependence upon ε in the notations for the sake of brevity.

The linearized flow $\partial_2\mathcal{E}_F$ is characterized by $\partial_2\mathcal{E}_F(t,u)w_0 = w$, where

$$i\varepsilon\partial_t w + \frac{\varepsilon^2}{2}\Delta w = f\left(|u|^2\right)w + f\left(\overline{u}w + u\overline{w}\right)u; \quad w_{|t=0} = w_0.$$

We note that it is not compatible with our approach, inasmuch as it *does not preserve the (monokinetic) WKB structure*: if $u = ae^{i\phi/\varepsilon}$ and $w_0 = b_0e^{i\varphi_0/\varepsilon}$, then the equation becomes

$$i\varepsilon\partial_t w + \frac{\varepsilon^2}{2}\Delta w = f\left(|a|^2\right)w + f\left(\overline{a}e^{-i\phi/\varepsilon}w + ae^{i\phi/\varepsilon}\overline{w}\right)ae^{i\phi/\varepsilon}; \quad w_{|t=0} = b_0e^{i\varphi_0/\varepsilon}.$$

In general, this is not compatible with a solution of the form

$$w = b^\varepsilon e^{i\varphi^\varepsilon/\varepsilon},$$

with b^ε and φ^ε uniformly bounded in Sobolev spaces. Possibly, w should rather be seeked as a superposition of WKB states,

$$w = \sum_j b_j^\varepsilon e^{i\varphi_j^\varepsilon/\varepsilon}.$$

Another, less technical, way to see that the local error should not be expected to be a single WKB state consists in going back to the definition. We have seen that the numerical solution remains of the form (at time $t_n = n\Delta t$) $u_n^\varepsilon(x) = a_n^\varepsilon(x)e^{i\phi_n^\varepsilon(x)/\varepsilon}$, while the exact solution is of the form (Proposition 3.2) $u^\varepsilon(t,x) = a^\varepsilon(t,x)e^{i\phi^\varepsilon(t,x)/\varepsilon}$. Thus the local error is

$$\mathcal{L}(t_n,u_0)(x) = a_n^\varepsilon(x)e^{i\phi_n^\varepsilon(x)/\varepsilon} - a^\varepsilon(t,x)e^{i\phi^\varepsilon(t,x)/\varepsilon},$$

and it is very unlikely that this can be factored out as

$$\mathcal{L}(t_n,u_0)(x) = \alpha_n^\varepsilon(x)e^{i\varphi_n^\varepsilon(x)/\varepsilon},$$

with α_n^ε and φ_n^ε uniformly bounded in Sobolev spaces (consider for instance the trivial example, $\mathcal{L} = \left(e^{ix_1/\varepsilon} - 1\right)e^{-|x|^2}$).

This aspect is another motivation for working with the system (2.3)–(2.2) instead of the standard one (1.4)–(1.6). We therefore consider the operators A and B defined by

$$A\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix}-\frac{1}{2}|\nabla\phi|^2\\ -\nabla\phi\cdot\nabla a - \frac{1}{2}a\Delta\phi + i\frac{\varepsilon}{2}\Delta a\end{pmatrix}, \quad B\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix}-f\left(|a|^2\right)\\ 0\end{pmatrix}. \tag{5.1}$$

We note that with this approach, neither A nor B is a linear operator.

Lemma 5.2. *Let A and B defined by* (5.1). *Their commutator is given by*

$$[A,B]\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix}\nabla\phi\cdot\nabla f\left(|a|^2\right) - \operatorname{div} f\left(|a|^2\nabla\phi\right) - \varepsilon\operatorname{div} f\left(\operatorname{Im}\left(\overline{a}\nabla a\right)\right)\\ \nabla a\cdot\nabla f\left(|a|^2\right) + \frac{1}{2}a\Delta f\left(|a|^2\right)\end{pmatrix}.$$

As a consequence, if $s > d/2$, $\|\nabla\phi\|_{H^{s+2}} \leqslant M$, $\|a\|_{H^{s+1}} \leqslant M$, *then there exists* $C = C(M)$ *independent of* $\varepsilon \in (0,1]$ *such that*

$$[A,B]\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix}\varphi\\ b\end{pmatrix}, \quad \textit{with} \left\{\begin{aligned} \|\varphi\|_{H^{s+2}} &\leqslant C\left(\|\nabla\phi\|_{H^{s+2}} + \|a\|_{H^{s+1}}\right),\\ \|b\|_{H^s} &\leqslant C\|a\|_{H^{s+1}}.\end{aligned}\right.$$

In particular,

$$\|\varphi\|_{L^\infty} \leqslant C\left(\|\nabla\phi\|_{H^{s+2}} + \|a\|_{H^{s+1}}\right).$$

Proof. By definition (see [13, Section 3]),

$$[A,B]v = A'(v)B(v) - B'(v)A(v).$$

We have, since f is linear in its argument,

$$\begin{aligned} A'\begin{pmatrix}\phi\\ a\end{pmatrix}\begin{pmatrix}\varphi\\ b\end{pmatrix} &= \begin{pmatrix} -\nabla\phi\cdot\nabla\varphi \\ -\nabla\phi\cdot\nabla b - \nabla\varphi\cdot\nabla a - \frac{1}{2}b\Delta\phi - \frac{1}{2}a\Delta\varphi + i\frac{\varepsilon}{2}\Delta b\end{pmatrix},\\ B'\begin{pmatrix}\phi\\ a\end{pmatrix}\begin{pmatrix}\varphi\\ b\end{pmatrix} &= \begin{pmatrix} -f\left(\overline{a}b + a\overline{b}\right)\\ 0\end{pmatrix} = \begin{pmatrix} -2f\left(\operatorname{Re}\left(\overline{a}b\right)\right)\\ 0\end{pmatrix}.\end{aligned}$$

We compute

$$B'\begin{pmatrix}\phi\\ a\end{pmatrix}A\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix} 2f\left(\operatorname{Re}\left(\overline{a}\nabla\phi\cdot\nabla a\right)\right) + f\left(|a|^2\Delta\phi\right) + \varepsilon f\left(\operatorname{Im}\left(\overline{a}\Delta a\right)\right)\\ 0\end{pmatrix}$$

The main point is then to notice the factorizations

$$2\operatorname{Re}\left(\overline{a}\nabla\phi\cdot\nabla a\right) + |a|^2\Delta\phi = \operatorname{div}\left(|a|^2\nabla\phi\right), \quad \operatorname{Im}\left(\overline{a}\Delta a\right) = \operatorname{div}\operatorname{Im}\left(\overline{a}\nabla a\right),$$

and to recall $\partial_j f(\rho) = f(\partial_j\rho)$, $1 \leqslant j \leqslant d$.

The estimates of the lemma then follow from the explicit formula for $[A,B]$, from the fact that $H^{s+2}(\mathbf{R}^d)$, $H^{s+1}(\mathbf{R}^d)$ and $H^s(\mathbf{R}^d)$ are Banach algebras, from (3.1), and from the embedding $H^{s+2} \hookrightarrow L^\infty$. □

We have the explicit formula

$$\mathcal{Y}_\varepsilon^t\begin{pmatrix}\phi\\ a\end{pmatrix} = \mathcal{E}_B\left(t, \begin{pmatrix}\phi\\ a\end{pmatrix}\right) = \begin{pmatrix}\phi - tf\left(|a|^2\right)\\ a\end{pmatrix},$$

and we readily infer

$$\partial_2\mathcal{E}_B\left(t, \begin{pmatrix}\phi\\ a\end{pmatrix}\right)\begin{pmatrix}\varphi\\ b\end{pmatrix} = \begin{pmatrix}\varphi - 2t\operatorname{Re} f\left(\overline{a}b\right)\\ b\end{pmatrix}. \tag{5.2}$$

Finally, we compute

$$\partial_2\mathcal{E}_F\left(t, \begin{pmatrix}\phi\\ a\end{pmatrix}\right)\begin{pmatrix}\varphi_0\\ b_0\end{pmatrix} = \begin{pmatrix}\varphi(t)\\ b(t)\end{pmatrix}, \quad \text{where}$$

$$\left\{\begin{aligned} &\partial_t\varphi + \nabla\phi\cdot\nabla\varphi + 2\operatorname{Re} f\left(\overline{a}b\right) = 0; \quad \varphi_{|t=0} = \varphi_0,\\ &\partial_t b + \nabla\phi\cdot\nabla b + \nabla\varphi\cdot\nabla a + \frac{1}{2}\left(b\Delta\phi + a\Delta\varphi\right) = i\frac{\varepsilon}{2}\Delta b; \quad b_{|t=0} = b_0.\end{aligned}\right. \tag{5.3}$$

Lemma 5.3. *Let* $s > d/2$. *Assume that* $(\nabla\phi, a) \in L^1(I; H^{s+2}\times H^{s+1})$, *where* $0 \in I$. *There exists* C *independent of* $\varepsilon \in (0,1]$ *such that if* $(\nabla\varphi_0, b_0) \in H^{s+1}\times H^s$, *the solution to* (5.3) *satisfies for all* $t \in I$,

$$\|b(t)\|_{H^s} + \|\nabla\varphi(t)\|_{H^{s+1}} \leqslant \left(\|b_0\|_{H^s} + \|\nabla\varphi_0\|_{H^{s+1}}\right)e^{C\int_0^t\left(\|a(\tau)\|_{H^{s+1}} + \|\nabla\phi(\tau)\|_{H^{s+2}}\right)d\tau}.$$

If in addition $\varphi_0 \in L^\infty$, *then*

$$\|\varphi(t)\|_{L^\infty} \leqslant \left(\|\varphi_0\|_{L^\infty} + \|b_0\|_{H^s} + \|\nabla\varphi_0\|_{H^{s+1}}\right) e^{C\int_0^t \left(\|a(\tau)\|_{H^{s+1}} + \|\nabla\phi(\tau)\|_{H^{s+2}}\right)d\tau}.$$

Proof. Set $w = \nabla\varphi$: (5.3) implies

$$\begin{cases} \partial_t w + \nabla\phi\cdot\nabla w + \nabla^2\phi\cdot w + 2\,\mathrm{Re}\,\nabla f\left(\overline{a}b\right) = 0; \quad w_{|t=0} = \nabla\varphi_0, \\ \partial_t b + \nabla\phi\cdot\nabla b + w\cdot\nabla a + \dfrac{1}{2}\left(b\Delta\phi + a\,\mathrm{div}\,w\right) = i\dfrac{\varepsilon}{2}\Delta b; \quad b_{|t=0} = b_0. \end{cases} \tag{5.4}$$

As in the proof of Proposition 3.2, the term $i\Delta b$ being skew-symmetric, it does not show up in energy estimates. Using Lemma 3.1, we have the estimate

$$\begin{aligned} \|w(t)\|_{H^{s+1}} + \|b(t)\|_{H^s} &\leqslant \|w_0\|_{H^{s+1}} + \|b_0\|_{H^s} \\ &\quad + C\int_0^t \left(\|\nabla\phi(\tau)\|_{H^{s+2}} + \|a(\tau)\|_{H^{s+1}}\right)\left(\|w(\tau)\|_{H^{s+1}} + \|b(\tau)\|_{H^s}\right)d\tau, \end{aligned}$$

and the first estimate of the lemma stems from Gronwall lemma.

The second estimate then follows from the first equation in (5.3) (integrated in time), and (3.2). □

Putting these estimates together, and using Theorem 5.1, we obtain a result which is crucial in the proof of Theorem 1.5:

Theorem 5.4 (Local error estimate for WKB states)**.** *Let* $s > d/2 + 1$ *and* $\mu > 0$. *Suppose that*

$$\|\nabla\phi^\varepsilon\|_{H^{s+1}} \leqslant \mu, \quad \|a^\varepsilon\|_{H^s} \leqslant \mu.$$

There exist $C, c_0 > 0$ *(depending on* μ*) independent of* $\varepsilon \in (0,1]$ *such that*

$$\mathcal{L}\left(t, \begin{pmatrix}\phi^\varepsilon\\ a^\varepsilon\end{pmatrix}\right) := \mathcal{Z}_\varepsilon^t\begin{pmatrix}\phi^\varepsilon\\ a^\varepsilon\end{pmatrix} - \mathcal{S}_\varepsilon^t\begin{pmatrix}\phi^\varepsilon\\ a^\varepsilon\end{pmatrix} = \begin{pmatrix}\Psi^\varepsilon(t)\\ A^\varepsilon(t)\end{pmatrix},$$

where A^ε *and* Ψ^ε *satisfy*

$$\|\nabla\Psi^\varepsilon(t)\|_{H^s} + \|A^\varepsilon(t)\|_{H^{s-1}} \leqslant Ct^2, \quad 0 \leqslant t \leqslant c_0.$$

If in addition $\|\phi^\varepsilon\|_{L^\infty} \leqslant \mu$, *then (up to increasing* C*)*

$$\|\Psi^\varepsilon(t)\|_{L^\infty} \leqslant Ct^2, \quad 0 \leqslant t \leqslant c_0.$$

Proof. Let $t \in [0,c]$, and fix τ_1, τ_2 such that $0 \leqslant \tau_2 \leqslant \tau_1 \leqslant t$. Introduce the following intermediary notations:

$$\begin{aligned} &\mathcal{E}_A\left(\tau_1, \begin{pmatrix}\phi^\varepsilon\\ a^\varepsilon\end{pmatrix}\right) = \begin{pmatrix}\phi_1^\varepsilon\\ a_1^\varepsilon\end{pmatrix}, \\ &\mathcal{E}_B\left(\tau_2, \begin{pmatrix}\phi_1^\varepsilon\\ a_1^\varepsilon\end{pmatrix}\right) = \begin{pmatrix}\phi_2^\varepsilon\\ a_2^\varepsilon\end{pmatrix}, \\ &[B,A]\begin{pmatrix}\phi_2^\varepsilon\\ a_2^\varepsilon\end{pmatrix} = \begin{pmatrix}\phi_3^\varepsilon\\ a_3^\varepsilon\end{pmatrix}, \\ &\partial_2\mathcal{E}_B\left(\tau_1 - \tau_2, \begin{pmatrix}\phi_1^\varepsilon\\ a_1^\varepsilon\end{pmatrix}\right)\begin{pmatrix}\phi_3^\varepsilon\\ a_3^\varepsilon\end{pmatrix} = \begin{pmatrix}\phi_4^\varepsilon\\ a_4^\varepsilon\end{pmatrix}, \\ &\mathcal{E}_B\left(\tau_1, \begin{pmatrix}\phi^\varepsilon\\ a^\varepsilon\end{pmatrix}\right) = \begin{pmatrix}\tilde{\phi}_1^\varepsilon\\ \tilde{a}_1^\varepsilon\end{pmatrix}, \\ &\mathcal{E}_A\left(\tau_1, \begin{pmatrix}\tilde{\phi}_1^\varepsilon\\ \tilde{a}_1^\varepsilon\end{pmatrix}\right) = \begin{pmatrix}\tilde{\phi}_2^\varepsilon\\ \tilde{a}_2^\varepsilon\end{pmatrix} \end{aligned}$$

Then in view of Theorem 5.1, we have

$$\begin{pmatrix}\Psi^\varepsilon\\ A^\varepsilon\end{pmatrix} = \int_0^t\int_0^{\tau_1} \partial_2\mathcal{E}_F\left(t-\tau_1, \begin{pmatrix}\tilde\phi_2^\varepsilon\\ \tilde a_2^\varepsilon\end{pmatrix}\right)\begin{pmatrix}\phi_4^\varepsilon\\ a_4^\varepsilon\end{pmatrix} d\tau_2 d\tau_1.$$

In view of Proposition 4.4, we have, uniformly on $[0,c]$, for c sufficiently small,

$$\|\nabla\phi_1^\varepsilon\|_{H^{s+1}} \leqslant 2\mu, \quad \|a_1^\varepsilon\|_{H^s} \leqslant 2\mu.$$

Now Lemma 4.1 implies (up to decreasing c)

$$\|\nabla\phi_2^\varepsilon\|_{H^{s+1}} \leqslant 3\mu, \quad \|a_2^\varepsilon\|_{H^s} \leqslant 3\mu.$$

From Lemma 5.2, we infer

$$\|\nabla\phi_3^\varepsilon\|_{H^{s}} \leqslant 4\mu, \quad \|a_3^\varepsilon\|_{H^{s-1}} \leqslant 4\mu,$$

provided that $s-1>d/2$. In view of (5.2), we have

$$a_4^\varepsilon = a_3^\varepsilon, \quad \phi_4^\varepsilon = \phi_3^\varepsilon - 2(\tau_1-\tau_2)\operatorname{Re} f\left(\overline{a}_1^\varepsilon a_3^\varepsilon\right),$$

and therefore

$$\|\nabla\phi_4^\varepsilon\|_{H^{s-1}} \leqslant 5\mu, \quad \|a_4^\varepsilon\|_{H^{s-1}} \leqslant 5\mu,$$

since $s-1>d/2$. Now Corollary 4.7 implies

$$\|\nabla\tilde\phi_2^\varepsilon\|_{H^{s+1}} \leqslant 4\mu, \quad \|\tilde a_2^\varepsilon\|_{H^s} \leqslant 4\mu.$$

Finally, Lemma 5.3 yields, up to decreasing c one last time,

$$\partial_2\mathcal{E}_F\left(t-\tau_1, \begin{pmatrix}\tilde\phi_2^\varepsilon\\ \tilde a_2^\varepsilon\end{pmatrix}\right)\begin{pmatrix}\phi_4^\varepsilon\\ a_4^\varepsilon\end{pmatrix} = \begin{pmatrix}\theta^\varepsilon\\ \alpha^\varepsilon\end{pmatrix}, \text{ with } \|\nabla\theta^\varepsilon\|_{H^s} \leqslant 10\mu, \quad \|\alpha^\varepsilon\|_{H^{s-1}} \leqslant 10\mu.$$

The first estimate of the theorem then follows by integrating with respect to (τ_1,τ_2) on $\{0\leqslant\tau_2\leqslant\tau_1\leqslant t\}$. The L^∞-estimate of the phase follows similarly. □

Back to the wave functions, we obtain an estimate similar to the one presented in [13, Section 4.2.2]:

Corollary 5.5. *Let $s>d/2+1$ and $\mu>0$. Let $\phi_0^\varepsilon\in L^\infty, a_0^\varepsilon\in H^s$ with*

$$\|\phi_0^\varepsilon\|_{L^\infty}\leqslant\mu, \quad \|\nabla\phi_0^\varepsilon\|_{H^{s+1}}\leqslant\mu, \quad \|a_0^\varepsilon\|_{H^s}\leqslant\mu.$$

There exist $C,c_0>0$ (depending on μ) independent of $\varepsilon\in(0,1]$ such that

$$\left\|Z_\varepsilon^t\left(a_0^\varepsilon e^{i\phi_t^\varepsilon/\varepsilon}\right) - S_\varepsilon^t\left(a_0^\varepsilon e^{i\phi_0^\varepsilon/\varepsilon}\right)\right\|_{L^2} \leqslant C\frac{t^2}{\varepsilon}, \quad 0\leqslant t\leqslant c_0.$$

Proof. We have $S_\varepsilon^t u_0^\varepsilon = a^\varepsilon(t)e^{i\phi^\varepsilon(t)/\varepsilon}$ where a^ε and ϕ^ε are given by Proposition 3.2, and

$$a_t^\varepsilon - a^\varepsilon(t) = A^\varepsilon(t), \quad \phi_t^\varepsilon - \phi^\varepsilon(t) = \Psi^\varepsilon(t),$$

where A^ε and Ψ^ε are given by Theorem 5.4. We compute, since $\|a^\varepsilon(t)\|_{L^2} = \|u^\varepsilon(t)\|_{L^2} = \|a_0^\varepsilon\|_{L^2}$,

$$\begin{aligned}\left\|Z_\varepsilon^t\left(a_0^\varepsilon e^{i\phi_t^\varepsilon/\varepsilon}\right) - S_\varepsilon^t u_0^\varepsilon\right\|_{L^2} &= \left\|a_t^\varepsilon(t)e^{i\phi_t^\varepsilon/\varepsilon} - a^\varepsilon(t)e^{i\phi^\varepsilon(t)/\varepsilon}\right\|_{L^2}\\ &\leqslant \|a_t^\varepsilon - a^\varepsilon(t)\|_{L^2} + \left\|a^\varepsilon(t)\left(e^{i\phi_t^\varepsilon/\varepsilon} - e^{i\phi^\varepsilon(t)/\varepsilon}\right)\right\|_{L^2}\\ &\leqslant \|A^\varepsilon(t)\|_{L^2} + \|a^\varepsilon(t)\|_{L^2}\left\|\frac{\phi_t^\varepsilon-\phi^\varepsilon(t)}{2\varepsilon}\right\|_{L^\infty}\\ &\leqslant Ct^2 + \frac{\mu}{2\varepsilon}\|\Psi^\varepsilon(t)\|_{L^\infty} \lesssim \frac{t^2}{\varepsilon},\end{aligned}$$

where we have used Theorem 5.4. □

Corollary 5.6 (Local error for quadratic observables)**.** *Let* $s > d/2 + 1$ *and* $\mu > 0$. *Let* $\phi^\varepsilon \in L^\infty, a^\varepsilon \in H^s$ *with*

$$\|\phi^\varepsilon\|_{L^\infty} \leqslant \mu, \quad \|\nabla\phi^\varepsilon\|_{H^{s+1}} \leqslant \mu, \quad \|a^\varepsilon\|_{H^s} \leqslant \mu.$$

There exist $C, c_0 > 0$ *independent of* $\varepsilon \in (0,1]$ *such that for* $0 \leqslant t \leqslant c_0$, *and* $u_0^\varepsilon = a_0^\varepsilon e^{i\phi_0^\varepsilon/\varepsilon}$,

$$\begin{aligned}&\left\| \left|Z_\varepsilon^t u_0^\varepsilon\right|^2 - \left|S_\varepsilon^t u_0^\varepsilon\right|^2 \right\|_{L^1(\mathbf{R}^d)\cap L^\infty(\mathbf{R}^d)} \leqslant Ct^2,\\ &\left\| \operatorname{Im}\left(\varepsilon \overline{Z_\varepsilon^t u_0^\varepsilon} \nabla Z_\varepsilon^t u_0^\varepsilon\right) - \operatorname{Im}\left(\varepsilon \overline{S_\varepsilon^t u_0^\varepsilon}\nabla S_\varepsilon^t u_0^\varepsilon\right)\right\|_{L^1(\mathbf{R}^d)\cap L^\infty(\mathbf{R}^d)} \leqslant Ct^2.\end{aligned}$$

Proof. Resuming the notations from the proof of Corollary 5.5, we have

$$\left|Z_\varepsilon^t u_0^\varepsilon\right|^2 - \left|S_\varepsilon^t u_0^\varepsilon\right|^2 = |a_t^\varepsilon|^2 - |a^\varepsilon(t)|^2,$$

and the Cauchy-Schwarz inequality yields

$$\left\||a_t^\varepsilon|^2 - |a^\varepsilon(t)|^2\right\|_{L^1} \leqslant \|a_t^\varepsilon - a^\varepsilon(t)\|_{L^2} \left(\|a_t^\varepsilon\|_{L^2} + \|a^\varepsilon(t)\|_{L^2}\right).$$

The first part of the corollary then stems from Theorem 5.4. Similarly,

$$\begin{aligned}\operatorname{Im}\left(\varepsilon \overline{Z_\varepsilon^t u_0^\varepsilon} \nabla Z_\varepsilon^t u_0^\varepsilon\right) - \operatorname{Im}\left(\varepsilon \overline{S_\varepsilon^t u_0^\varepsilon}\nabla S_\varepsilon^t u_0^\varepsilon\right) &= |a_t^\varepsilon|^2 \nabla\phi_t^\varepsilon - |a^\varepsilon(t)|^2\nabla\phi^\varepsilon(t)\\ &\quad + \varepsilon \operatorname{Im}\left(\overline{a_t^\varepsilon}\nabla a_t^\varepsilon\right) - \varepsilon\operatorname{Im}\left(\overline{a^\varepsilon(t)}\nabla a^\varepsilon(t)\right).\end{aligned}$$

The second part of the corollary then follows easily from Hölder inequality and Theorem 5.4. □

6. End of the proof of Theorem 1.5

6.1. Lady Windermere's fan.

We denote

$$\begin{pmatrix}\phi_n^\varepsilon\\ a_n^\varepsilon\end{pmatrix} = \left(\mathcal{Z}_\varepsilon^{\Delta t}\right)^n \begin{pmatrix}\phi_0\\ a_0\end{pmatrix}.$$

To prove Theorem 1.5, we rephrase it in a more precise way:

Proposition 6.1. *Let* $s > d/2 + 2$, $\phi_0 \in L^\infty, a_0 \in H^s$, *with* $\nabla\phi_0 \in H^{s+1}$, *and* T *as in Theorem 1.5. There exist* $\nu, \gamma, \Delta t_0, c_1, C_0 > 0$ *such that for all* $\varepsilon \in (0,1]$, *all* $0 \leqslant \Delta t \leqslant \Delta t_0$ *and all* $n \in \mathbf{N}$ *such that* $t_n = n\Delta t \in [0,T]$,

$$\|\nabla\phi_n^\varepsilon\|_{H^s} + \|a_n^\varepsilon\|_{H^{s-1}} \leqslant \nu, \tag{6.1}$$

$$\|\nabla\phi_n^\varepsilon - \nabla\phi^\varepsilon(t_n)\|_{H^s} + \|a_n^\varepsilon - a^\varepsilon(t_n)\|_{H^{s-1}} \leqslant \gamma\Delta t, \tag{6.2}$$

$$\|\nabla\phi_n^\varepsilon\|_{H^{s+1}} + \|a_n^\varepsilon\|_{H^s} \leqslant e^{c_1\nu n\Delta t} \leqslant C_0 = e^{c_1\nu T}, \tag{6.3}$$

$$\|\phi_n^\varepsilon - \phi^\varepsilon(t_n)\|_{L^\infty} \leqslant \gamma\Delta t. \tag{6.4}$$

Remark 6.2 (L^∞ bounds). The above result has an important technical consequence: the numerical solution $u_n^\varepsilon = a_n^\varepsilon e^{i\phi_n^\varepsilon/\varepsilon}$ is uniformly bounded in $L^\infty(\mathbf{R}^d)$. In view of Proposition 3.2, the same holds for the exact solution $u^\varepsilon(t)$. Such informations are very delicate to obtain in general. Even in one dimension, the Gagliardo-Nirenberg inequality

$$\|u^\varepsilon\|_{L^\infty} \leqslant \sqrt{2}\|u^\varepsilon\|_{L^2}^{1/2}\|\partial_x u^\varepsilon\|_{L^2}^{1/2}$$

would not yield better than $\|u^\varepsilon\|_{L^\infty} \lesssim \varepsilon^{-1/2}$, because of the rapid oscillations present in u^ε ($\phi^\varepsilon \neq 0$). Here, the uniform L^∞ estimates follow from the fact that a WKB regime is considered.

Proof. The proof that we present follows essentially the lines of [17, Section 5]. Denote by $\begin{pmatrix}\phi_k\\ a_k\end{pmatrix} = \left(\mathcal{Z}_L^{\Delta t}\right)^k \begin{pmatrix}\phi_0\\ a_0\end{pmatrix}$ the numerical solution, and

$$\begin{pmatrix}\phi_n^k\\ a_n^k\end{pmatrix} = \mathcal{S}^{(n-k)\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}.$$

In this proof, we omit the dependence of all the functions with respect to ε. From Proposition 3.2, there exists R such that

$$\left\|\begin{pmatrix}\phi(t)\\ a(t)\end{pmatrix}\right\|_{\nabla H^{s+1}\times H^s} := \|\nabla\phi(t)\|_{H^{s+1}} + \|a(t)\|_{H^s} \leqslant R, \quad \forall t\in[0,T].$$

We prove Proposition 6.1 by induction, with $\nu = R+\delta$, $\delta>0$ so that the solution to (1.12) with data in the ball characterized by (6.1) remains smooth up to time T (this is possible, since $T<T_{\max}$). The estimates are obviously satisfied for $n=0$. Let $n\geqslant 1$, and suppose that the induction assumption is true for $0\leqslant k\leqslant n-1$. We introduce the same telescopic series as in [17], which is different from (1.10), the latter being useful mostly when the problem (hence the splitting operator) is linear:

$$\begin{pmatrix}\phi_n^\varepsilon\\ a_n^\varepsilon\end{pmatrix} - \begin{pmatrix}\phi^\varepsilon(t_n)\\ a^\varepsilon(t_n)\end{pmatrix} = \sum_{j=0}^{n-1}\left(\mathcal{S}_\varepsilon^{(n-j-1)\Delta t}\mathcal{Z}_\varepsilon^{\Delta t}\begin{pmatrix}\phi_j^\varepsilon\\ a_j^\varepsilon\end{pmatrix} - \mathcal{S}_\varepsilon^{(n-j-1)\Delta t}\mathcal{S}_\varepsilon^{\Delta t}\begin{pmatrix}\phi_j^\varepsilon\\ a_j^\varepsilon\end{pmatrix}\right). \tag{6.5}$$

Noting the properties $f_n = f_n^n$ and $f(t_n) = f_n^0$ ($f=\phi$ or a), we estimate

$$\begin{aligned}\|\nabla\phi_n - &\nabla\phi(t_n)\|_{H^s} + \|a_n - a(t_n)\|_{H^{s-1}}\\ &\leqslant \sum_{k=0}^{n-1}\left(\|\nabla\phi_n^{k+1} - \nabla\phi_n^k\|_{H^s} + \|a_n^{k+1} - a_n^k\|_{H^{s-1}}\right)\\ &\leqslant \sum_{k=0}^{n-1}\left\|\mathcal{S}^{(n-k-1)\Delta t}\left(\mathcal{Z}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}\right) - \mathcal{S}^{(n-k-1)\Delta t}\left(\mathcal{S}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}\right)\right\|_{\nabla H^s\times H^{s-1}}.\end{aligned}$$

For $k\leqslant n-2$, $\mathcal{Z}_L^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix} = \begin{pmatrix}\phi_{k+1}\\ a_{k+1}\end{pmatrix}$ and Proposition 3.3 yields, along with the induction assumption (all the norms are in $\nabla H^s\times H^{s-1}$),

$$\begin{aligned}\left\|\mathcal{S}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}\right\| &\leqslant \left\|\mathcal{S}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix} - \mathcal{S}^{\Delta t}\begin{pmatrix}\phi(t_k)\\ a(t_k)\end{pmatrix}\right\| + \left\|\mathcal{S}^{\Delta t}\begin{pmatrix}\phi(t_k)\\ a(t_k)\end{pmatrix}\right\|\\ &\leqslant K(2R)\left\|\begin{pmatrix}\phi_k\\ a_k\end{pmatrix} - \begin{pmatrix}\phi(t_k)\\ a(t_k)\end{pmatrix}\right\| + \left\|\begin{pmatrix}\phi(t_{k+1})\\ a(t_{k+1})\end{pmatrix}\right\|\\ &\leqslant K\gamma\Delta t + R,\end{aligned}$$

which is bounded by $R+\delta$ if $0<\Delta t\leqslant \Delta t_0 \ll 1$. Up to replacing K with $\max(K,1)$, we obtain that, for $k\leqslant n-1$ and $n\Delta t\leqslant T$,

$$\left\|\mathcal{S}^{(n-k-1)\Delta t}\left(\mathcal{Z}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}\right) - \mathcal{S}^{(n-k-1)\Delta t}\left(\mathcal{S}^{\Delta t}\begin{pmatrix}\phi_k\\ a_k\end{pmatrix}\right)\right\|_{\nabla H^s\times H^{s-1}}$$

is controlled by

$$K \left\| \mathcal{Z}^{\Delta t} \begin{pmatrix} \phi_k \\ a_k \end{pmatrix} - \mathcal{S}^{\Delta t} \begin{pmatrix} \phi_k \\ a_k \end{pmatrix} \right\|_{\nabla H^s \times H^{s-1}} .$$

Using the local error estimate from Theorem 5.4, we infer, using (6.3),

$$\left\| \mathcal{S}^{(n-k-1)\Delta t} \left(\mathcal{Z}^{\Delta t} \begin{pmatrix} \phi_k \\ a_k \end{pmatrix} \right) - \mathcal{S}^{(n-k-1)\Delta t} \left(\mathcal{S}^{\Delta t} \begin{pmatrix} \phi_k \\ a_k \end{pmatrix} \right) \right\|_{H^{s-5}} \leqslant CK \left(\Delta t\right)^2 ,$$

for some uniform constant C depending on C_0. Therefore,

$$\|\nabla \phi_n - \nabla \phi(t_n)\|_{H^s} + \|a_n - a(t_n)\|_{H^{s-1}} \leqslant CTK\Delta t,$$

and we can take $\gamma = CTK$, which is uniform in n and Δt, in order to get (6.1) and (6.2). Then (6.3) follows from Corollary 4.8, in view of (6.1) and Sobolev embedding, since we have assumed $s > d/2+2$. Finally, the L^∞-estimates (6.4) for ϕ_n^ε are now straightforward (up to increasing γ), and are left out. $\square$

Remark 6.3 (Nonlinear Schrödinger equation). We can now explain why Assumption 1.2 is needed for the complete argument to work out. If we wanted to prove the analogue of Theorem 1.5 for, say, the defocusing cubic Schrödinger equation

$$i\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\Delta u^\varepsilon = |u^\varepsilon|^2 u^\varepsilon,$$

then many results would still be available. In terms of the numerical scheme, the only change would affect the operator $\mathcal{Y}_\varepsilon^t$: (2.2) would be replaced by

$$\begin{cases} \partial_t \phi^\varepsilon + |a^\varepsilon|^2 = 0; \quad \phi^\varepsilon_{|t=0} = \phi_0^\varepsilon, \\ \partial_t a^\varepsilon = 0; \quad a^\varepsilon_{|t=0} = a_0^\varepsilon. \end{cases}$$

Working in H^s for $s > d/2$, we see that unlike what happens under Assumption 1.2, ϕ^ε cannot be more regular than a_0^ε. On the other hand, the WKB formulation of the free Schrödinger flow (2.3) induces a shift of regularity: if ϕ^ε is in H^s for s large, then a^ε must not be expected to be more regular than H^{s-2}. Therefore, the splitting operator $\mathcal{Z}_\varepsilon^t$ induces a loss of regularity, and this loss is iterated like $T/\Delta t$ times. It is this aspect which makes it hard to adapt Proposition 6.1 to the case of the nonlinear Schrödinger equation.

6.2. **Proof of Corollary 1.6.**

Once Theorem 1.5 is available, we simply write, like in the proof of Corollary 5.5,

$$\begin{aligned} \left(Z_\varepsilon^{\Delta t}\right)^n u_0^\varepsilon - S_\varepsilon^{t_n} u_0^\varepsilon &= a_n^\varepsilon e^{i\phi_n^\varepsilon/\varepsilon} - a^\varepsilon(t_n) e^{i\phi^\varepsilon(t_n)/\varepsilon} \\ &= \left(a_n^\varepsilon - a^\varepsilon(t_n)\right) e^{i\phi_n^\varepsilon/\varepsilon} + a^\varepsilon(t_n)\left(e^{i\phi_n^\varepsilon/\varepsilon} - e^{i\phi^\varepsilon(t_n)/\varepsilon}\right). \end{aligned}$$

Taking the L^2-norm, we infer

$$\left\| \left(Z_\varepsilon^{\Delta t}\right)^n u_0^\varepsilon - S_\varepsilon^{t_n} u_0^\varepsilon \right\|_{L^2} \leqslant \|a_n^\varepsilon - a^\varepsilon(t_n)\|_{L^2} + \|a^\varepsilon(t_n)\|_{L^2} \left\| \frac{\phi_n^\varepsilon - \phi^\varepsilon(t_n)}{\varepsilon} \right\|_{L^\infty},$$

and Corollary 1.6 is a direct consequence of Theorem 1.5.

6.3. **Proof of Corollary 1.7.**

Corollary 1.7 also stems directly from Theorem 1.5, by resuming the same computations as in the proof of Corollary 5.6.

7. Weakly nonlinear regime

We now consider (1.1) in the case $\alpha \geqslant 1$, under Assumption 1.8 on the nonlinearity. In view of the formal computations presented in Section 1.2, the case $\alpha = 1$ can be considered as the only interesting one, since no nonlinear effect is expected at leading order when $\alpha > 1$. Since it is possible to treat both cases at once, we take advantage of this opportunity.

The analysis in the case $\alpha \geqslant 1$ being quite easier than in the case $\alpha = 0$ (even under Assumption 1.2, which is weaker than Assumption 1.8), we shall simply underline the modifications to be made in order to prove Proposition 1.10 by following the same steps as in the proof of Theorem 1.5.

To characterize the exact flow in terms of WKB states, (2.6) is replaced by

$$\begin{cases} \partial_t \phi^\varepsilon + \dfrac{1}{2}|\nabla \phi^\varepsilon|^2 = 0; \quad \phi^\varepsilon_{|t=0} = \phi_0, \\ \partial_t a^\varepsilon + \nabla \phi^\varepsilon \cdot \nabla a^\varepsilon + \dfrac{1}{2} a^\varepsilon \Delta \phi^\varepsilon = i\dfrac{\varepsilon}{2}\Delta a^\varepsilon - i\varepsilon^{\alpha-1} f\left(|a^\varepsilon|^2\right) a^\varepsilon; \quad a^\varepsilon_{|t=0} = a_0. \end{cases} \tag{7.1}$$

Thanks to the assumption $\alpha \geqslant 1$, the last term in the equation for a^ε is not singular as $\varepsilon \to 0$. More importantly, this is no longer a coupled system: the first equation is an eikonal equation, which we have analyzed in Section 4.2.

In the numerical scheme, the operator $\mathcal{X}^t_\varepsilon$, corresponding to the free Schrödinger flow, is the same as before, and analyzed in Section 4.2. On the other hand the operator $\mathcal{Y}^t_\varepsilon$ can be modified, since the nonlinearity does not affect the rapid oscillations (as can be seen also from (7.1)). We recall that we now consider

$$\begin{cases} \partial_t \phi^\varepsilon = 0; \quad \phi^\varepsilon_{|t=0} = \phi^\varepsilon_0, \\ \partial_t a^\varepsilon = -i\varepsilon^{\alpha-1} f\left(|a^\varepsilon|^2\right) a^\varepsilon; \quad a^\varepsilon_{|t=0} = a^\varepsilon_0. \end{cases}$$

We see that the possible loss of regularity pointed out in Remark 6.3 is not present here, since the regularity of ϕ^ε is not affected by the regularity of a^ε. Also, working with a^ε in H^s for $s > d/2$ ensures that the analysis of Section 4.2 can easily be adapted under Assumption 1.8, since $a^\varepsilon(t) = a^\varepsilon_0 \exp\left(-i\varepsilon^{\alpha-1} t f(|a^\varepsilon_0|^2)\right)$.

The main modification in the analysis concerns the local error estimate, since the statement of Lemma 5.2 must be revised. The operator A remains unchanged, and the operator B becomes

$$B\begin{pmatrix}\phi \\ a\end{pmatrix} = \begin{pmatrix} 0 \\ -i\varepsilon^{\alpha-1} f\left(|a|^2\right) a\end{pmatrix}.$$

We compute successively

$$B'\begin{pmatrix}\phi \\ a\end{pmatrix}\begin{pmatrix}\varphi \\ b\end{pmatrix} = -i\varepsilon^{\alpha-1}\begin{pmatrix} 0 \\ 2f_1\left(\operatorname{Re}\left(\overline{a}b\right)\right)a + f_1\left(|a|^2\right)b + 2f_2'\left(|a|^2\right)\operatorname{Re}\left(\overline{a}b\right)\end{pmatrix},$$

and

$$[A,B]\begin{pmatrix}\phi \\ a\end{pmatrix} = i\varepsilon^{\alpha-1}\begin{pmatrix} 0 \\ F(\phi,a)\end{pmatrix},$$

where

$$\begin{aligned} F(\phi,a) = {} & \nabla\phi \cdot \nabla\left(f\left(|a|^2\right)a\right) + \frac{1}{2} f\left(|a|^2\right) a \Delta\phi - i\frac{\varepsilon}{2}\Delta\left(f\left(|a|^2\right)a\right) \\ & - a \operatorname{div} f_1\left(|a|^2 \nabla\phi\right) - \varepsilon a \operatorname{div} f_1\left(\operatorname{Im}\left(\overline{a}\nabla a\right)\right) \\ & - f_2'\left(|a|^2\right)\operatorname{div}\left(|a|^2\nabla\phi + \varepsilon \operatorname{Im}\left(\overline{a}\nabla a\right)\right). \end{aligned}$$

The main point to notice is that if $s > d/2 + 2$, then F maps $H^s \times H^s$ to H^{s-2}. Proposition 1.10 then follows by resuming the same steps as in the proof of Proposition 6.1.

Appendix A. Linear Schrödinger equation

Consider the (linear) Schrödinger equation with a potential,

$$i\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\Delta u^\varepsilon = Vu^\varepsilon; \quad u^\varepsilon_{|t=0} = u_0^\varepsilon, \tag{A.1}$$

with $V = V(t,x) \in \mathbf{R}$. We assume that V grows at most quadratically in space:

Assumption A.1. *$V \in L^\infty_{\rm loc}([0,\infty) \times \mathbf{R}^d)$ is real-valued, and smooth with respect to the space variable: for (almost) all $t \geqslant 0$, $x \mapsto V(t,x)$ is a C^∞ map. Moreover, it is at most quadratic in space:*

$$\forall \alpha \in \mathbf{N}^d,\ |\alpha| \geqslant 2,\ \forall T > 0, \quad \partial_x^\alpha V \in L^\infty([0,T] \times \mathbf{R}^d).$$

In addition, $t \mapsto V(t,0)$ belongs to $L^\infty_{\rm loc}([0,\infty))$.

Then for $u_0^\varepsilon \in L^2(\mathbf{R}^d)$, (A.1) has a unique solution $u^\varepsilon \in C([0,\infty); L^2(\mathbf{R}^d))$, and its L^2-norm is conserved, $\|u^\varepsilon(t)\|_{L^2} = \|u_0^\varepsilon\|_{L^2}$ for all $t \geqslant 0$; see e.g. [14]. The following result is standard in semi-classical analysis (see e.g. [26]). We sketch the proof for completeness.

Proposition A.2. *Let $k \in \mathbf{N}$, V satisfying Assumption A.1, and $u_0^\varepsilon \in L^2(\mathbf{R}^d)$. Suppose in addition that u_0^ε satisfies*

$$\|u_0^\varepsilon\|_{\Sigma^k_\varepsilon} := \sup_{0<\varepsilon\leqslant 1} \left(\|u_0^\varepsilon\|_{L^2} + \||x|^k u_0^\varepsilon\|_{L^2} + \||\varepsilon\nabla|^k u_0^\varepsilon\|_{L^2} \right) < \infty. \tag{A.2}$$

Then for all $T > 0$, the solution to (A.1) *satisfies*

$$\sup_{0<\varepsilon\leqslant 1} \sup_{t\in[0,T]} \left(\|u^\varepsilon(t)\|_{L^2} + \||x|^k u^\varepsilon(t)\|_{L^2} + \||\varepsilon\nabla|^k u^\varepsilon(t)\|_{L^2} \right) < \infty.$$

Proof. The key point is that the functions $\varepsilon\nabla u^\varepsilon$ and xu^ε satisfy a closed system of estimates. Indeed, $\varepsilon\nabla$ does not commute with the equation, and $\varepsilon\nabla u^\varepsilon$ satisfies

$$i\varepsilon\partial_t \left(\varepsilon\nabla u^\varepsilon\right) + \frac{\varepsilon^2}{2}\Delta\left(\varepsilon\nabla u^\varepsilon\right) = V\varepsilon\nabla u^\varepsilon + \left(\varepsilon\nabla V\right) u^\varepsilon.$$

Similarly,

$$i\varepsilon\partial_t \left(xu^\varepsilon\right) + \frac{\varepsilon^2}{2}\Delta\left(xu^\varepsilon\right) = Vxu^\varepsilon + \varepsilon^2\nabla u^\varepsilon.$$

The standard L^2 estimate then yields

$$\|\varepsilon\nabla u^\varepsilon(t)\|_{L^2} \leqslant \|\varepsilon\nabla u_0^\varepsilon\|_{L^2} + \int_0^t \|(\nabla V)u^\varepsilon(\tau)\|_{L^2} d\tau,$$

$$\|xu^\varepsilon(t)\|_{L^2} \leqslant \|xu_0^\varepsilon\|_{L^2} + \int_0^t \|\varepsilon\nabla u^\varepsilon(\tau)\|_{L^2} d\tau.$$

Now under Assumption A.1, for $T > 0$ fixed, we have the pointwise estimate

$$|\nabla V(\tau,x) u^\varepsilon(\tau,x)| \leqslant C(T)\left(1+|x|\right)|u^\varepsilon(\tau,x)|, \quad 0 \leqslant \tau \leqslant T.$$

Recalling that the L^2-norm of u^ε is bounded, Gronwall lemma, applied to

$$y(t) = \|\varepsilon\nabla u^\varepsilon(t)\|_{L^2} + \|xu^\varepsilon(t)\|_{L^2},$$

yields the proposition in the case $k = 1$. The general case follows by induction. □

Example A.3. If u_0^ε is of WKB type (1.2), or more generally (2.1), with ϕ_0 at most quadratic (in the sense of Assumption A.1), and $a_0 \in H^k \cap \mathcal{F}(H^k)$, then the above assumptions are fulfilled. Note however that Proposition A.2 is valid for all time, and in particular after the formation of caustics, if any.

Example A.4. If

$$u_0^\varepsilon(x) = \frac{1}{\varepsilon^{\theta d/2}} a_0\left(\frac{x-q}{\varepsilon^\theta}\right) e^{i(x-q)\cdot p/\varepsilon},$$

with $q, p \in \mathbf{R}^d$, $\theta \in [0,1]$, and $a_0 \in \mathcal{S}(\mathbf{R}^d)$, then again, Proposition A.2 is valid for all time. If $\theta = 0$, this datum is a particular WKB datum (with a linear phase). If $\theta = 1/2$, this means that an initial coherent state is considered (see e.g. [11]). If $\theta = 1$, the initial datum is concentrating at point q, which corresponds to a caustic reduced to one point (focal point; see [7]).

Recall that if the splitting operators are defined by

$$A = i\frac{\varepsilon}{2}\Delta; \quad B = -\frac{i}{\varepsilon}V,$$

then their Lie commutator is given by

$$[A, B] = \nabla V \cdot \nabla + \frac{1}{2}\Delta V.$$

With the norm $\|u\|_{\Sigma_\varepsilon^2}$ defined in (A.2), note the control

$$\|\varepsilon \nabla V \cdot \nabla u\|_{L^2} \lesssim \|u\|_{\Sigma_\varepsilon^2},$$

which follows from Assumption A.1. By working with the norm $\|u\|_{\Sigma_\varepsilon^2}$, rather than with the norm $\|u\|_{H_\varepsilon^1}$ defined in Section 1.1, and used in [3, 12], the following result is a direct consequence of [12] and Proposition A.2:

Proposition A.5. *Let $d \geqslant 1$, and V satisfying Assumption A.1. Suppose that $\|u_0^\varepsilon\|_{\Sigma_\varepsilon^2} < \infty$. Then for all $T > 0$, there exist C, c_0 independent of $\varepsilon \in (0,1]$ such that for all $\Delta t \in (0, c_0]$, for all $n \in \mathbf{N}$ such that $n\Delta t \in [0,T]$,*

$$\left\| \left(Z_\varepsilon^{\Delta t}\right)^n u_0^\varepsilon - S_\varepsilon^{t_n} u_0^\varepsilon \right\|_{L^2(\mathbf{R}^d)} \leqslant C\frac{\Delta t}{\varepsilon},$$

where $S_\varepsilon^t u_0^\varepsilon = u^\varepsilon(t)$ in (A.1), *and $Z_\varepsilon^t = e^{tB}e^{tA}$.*

Acknowledgements. The author is grateful to Christophe Besse and Stéphane Descombes for precious references, and to the referees and to Luca Dieci as an editor, for their constructive remarks.

References

[1] T. Alazard and R. Carles, *Semi-classical limit of Schrödinger–Poisson equations in space dimension $n \geqslant 3$*, J. Differential Equations, 233 (2007), pp. 241–275.

[2] S. Alinhac and P. Gérard, *Pseudo-differential operators and the Nash-Moser theorem*, vol. 82 of Graduate Studies in Mathematics, American Mathematical Society, Providence, RI, 2007. Translated from the 1991 French original by Stephen S. Wilson.

[3] W. Bao, S. Jin, and P. A. Markowich, *On time-splitting spectral approximations for the Schrödinger equation in the semiclassical regime*, J. Comput. Phys., 175 (2002), pp. 487–524.

[4] ———, *Numerical study of time-splitting spectral discretizations of nonlinear Schrödinger equations in the semiclassical regimes*, SIAM J. Sci. Comput., 25 (2003), pp. 27–64.

[5] C. Besse, B. Bidégaray, and S. Descombes, *Order estimates in time of splitting methods for the nonlinear Schrödinger equation*, SIAM J. Numer. Anal., 40 (2002), pp. 26–40.

[6] F. Brezzi and P. A. Markowich, *The three-dimensional Wigner-Poisson problem: existence, uniqueness and approximation*, Math. Methods Appl. Sci., 14 (1991), pp. 35–61.

[7] R. Carles, *Semi-classical analysis for nonlinear Schrödinger equations*, World Scientific Publishing Co. Pte. Ltd., Hackensack, NJ, 2008.

[8] R. Carles, R. Danchin, and J.-C. Saut, *Madelung, Gross-Pitaevskii and Korteweg*, Nonlinearity, 25 (2012), pp. 2843–2873.

[9] R. Carles and B. Mohammadi, *Numerical aspects of the nonlinear Schrödinger equation in the semiclassical limit in a supercritical regime*, ESAIM Math. Model. Numer. Anal., 45 (2011), pp. 981–1008.

[10] T. Cazenave, *Semilinear Schrödinger equations*, vol. 10 of Courant Lecture Notes in Mathematics, New York University Courant Institute of Mathematical Sciences, New York, 2003.

[11] M. Combescure and D. Robert, *Semiclassical spreading of quantum wave packets and applications near unstable fixed points of the classical flow*, Asymptot. Anal., 14 (1997), pp. 377–404.

[12] S. Descombes and M. Thalhammer, *An exact local error representation of exponential operator splitting methods for evolutionary problems and applications to linear Schrödinger equations in the semi-classical regime*, BIT, 50 (2010), pp. 729–749.

[13] ———, *The Lie–Trotter splitting for nonlinear evolutionary problems with critical parameters. A compact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime*, IMA J. Numer. Anal., 33 (2013), pp. 722–745.

[14] D. Fujiwara, *Remarks on the convergence of the Feynman path integrals*, Duke Math. J., 47 (1980), pp. 559–600.

[15] P. Gamblin, *Solution régulière à temps petit pour l'équation d'Euler-Poisson*, Comm. Partial Differential Equations, 18 (1993), pp. 731–745.

[16] E. Grenier, *Semiclassical limit of the nonlinear Schrödinger equation in small time*, Proc. Amer. Math. Soc., 126 (1998), pp. 523–530.

[17] H. Holden, C. Lubich, and N. H. Risebro, *Operator splitting for partial differential equations with Burgers nonlinearity*, Math. Comp., 82 (2013), pp. 173–185.

[18] S. Jin, P. Markowich, and C. Sparber, *Mathematical and computational methods for semiclassical Schrödinger equations*, Acta Numer., 20 (2011), pp. 121–209.

[19] T. Kato and G. Ponce, *Commutator estimates and the Euler and Navier-Stokes equations*, Comm. Pure Appl. Math., 41 (1988), pp. 891–907.

[20] H. Li and C.-K. Lin, *Semiclassical limit and well-posedness of nonlinear Schrödinger-Poisson systems*, Electron. J. Differential Equations, (2003), pp. No. 93, 17 pp. (electronic).

[21] H. Liu and E. Tadmor, *Semiclassical limit of the nonlinear Schrödinger-Poisson equation with subcritical initial data*, Methods Appl. Anal., 9 (2002), pp. 517–531.

[22] C. Lubich, *On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations*, Math. Comp., 77 (2008), pp. 2141–2153.

[23] P. A. Markowich, P. Pietra, and C. Pohl, *Numerical approximation of quadratic observables of Schrödinger-type equations in the semi-classical limit*, Numer. Math., 81 (1999), pp. 595–630.

[24] S. Masaki, *Local existence and WKB approximation of solutions to Schrödinger-Poisson system in the two-dimensional whole space*, Comm. Partial Differential Equations, 35 (2010), pp. 2253–2278.

[25] ———, *Energy solution to a Schrödinger-Poisson system in the two-dimensional whole space*, SIAM J. Math. Anal., 43 (2011), pp. 2719–2731.

[26] D. Robert, *Autour de l'approximation semi-classique*, vol. 68 of Progress in Mathematics, Birkhäuser Boston Inc., Boston, MA, 1987.

[27] P. Zhang, *Wigner measure and the semiclassical limit of Schrödinger-Poisson equations*, SIAM J. Math. Anal., 34 (2002), pp. 700–718.

CNRS & Univ. Montpellier 2, Mathématiques, CC 051, 34095 Montpellier, France
E-mail address: `Remi.Carles@math.cnrs.fr`