On time splitting for NLS in the semiclassical regime

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with $u : [0, T] \times \mathbb{R}^d \to \mathbb{C}$, and $f : \mathbb{R}_+ \to \mathbb{R}$.

Splitting: solve successively two parts of the equation.

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$$i\partial_t u + \frac{1}{2}\Delta u = 0.$$

Same thing, thanks to Fourier (in space):

$$i\partial_t \widehat{u} - \frac{|\xi|^2}{2}\widehat{u} = 0.$$

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Splitting scheme(s)

Denote by X^t the linear flow: $X^t u_0 = u(t)$, where

$$i\partial_t u + \frac{1}{2}\Delta u = 0 \quad ; \quad u_{|t=0} = u_0,$$

and by Y^t the "nonlinear" flow: $Y^t u_0 = u(t)$, where

$$i\partial_t u = f\left(|u|^2\right) u \quad ; \quad u_{|t=0} = u_0.$$

- Lie-Trotter: $Z_L^{\Delta t} = Y^{\Delta t} \circ X^{\Delta t}$ or $Z_L^{\Delta t} = X^{\Delta t} \circ Y^{\Delta t}$.
- Strang: $Z_S^{\Delta t} = X^{\Delta t/2} \circ Y^{\Delta t} \circ X^{\Delta t/2}$ or $(\dots)$.
- Higher order...

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Convergence of the approximation

$$i\partial_t u + \frac{1}{2}\Delta u = |u|^2 u \quad ; \quad u_{|t=0} = u_0.$$

Theorem (Besse-Bidégaray-Descombes 02; Lubich 08)

Case $d \leqslant 2$: for $u_0 \in H^2(\mathbb{R}^d)$ and all $T > 0$, $\exists C, h_0$ such as if $\Delta t \in]0, h_0]$, $\forall n \in \mathbb{N}$ with $n\Delta t \in [0, T]$,

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

with $m_j = \max_{0 \leqslant t \leqslant T} \|u(t)\|_{H^j(\mathbb{R}^d)}$. If $d = 3$ and $u_0 \in H^4(\mathbb{R}^d)$,

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

Semiclassical regime

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

and $\varepsilon \to 0$. Initial datum of WKB type: $u_0^\varepsilon(0,x) = a_0(x)e^{i\phi_0(x)/\varepsilon}$.
Conserved quantities:

Mass: $\frac{d}{dt}\|u^\varepsilon(t)\|_{L^2}^2 = 0.$

Energy: $\frac{d}{dt}\left(\|\varepsilon\nabla u^\varepsilon(t)\|_{L^2}^2 + \int_{\mathbb{R}^d} F\left(|u^\varepsilon(t,x)|^2\right)dx\right) = 0.$

$\rightsquigarrow \|u^\varepsilon\|_{H^1} \approx \varepsilon^{-1}$. More generally, $m_j = \mathcal{O}(\varepsilon^{-j})$ (sharp).
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Hydrodynamics

$$i\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\Delta u^\varepsilon = f\left(|u^\varepsilon|^2\right) u^\varepsilon \quad ; \quad u_0^\varepsilon(0,x) = a_0(x)e^{i\phi_0(x)/\varepsilon}.$$

WKB type approximation: $u^\varepsilon(t,x) \approx a(t,x)e^{i\phi(t,x)/\varepsilon}$.

Position density: $\rho^\varepsilon(t,x) = |u^\varepsilon(t,x)|^2$.

Current density: $J^\varepsilon(t,x) = \varepsilon \operatorname{Im}\left(\overline{u}^\varepsilon(t,x)\nabla u^\varepsilon(t,x)\right)$.

Formally (justifications exist), ρ^ε and J^ε converge to:

$$\begin{cases} \partial_t\rho + \operatorname{div} J = 0 \quad ; \quad \rho_{|t=0} = |a_0|^2, \\ \partial_t J + \operatorname{div}\left(\dfrac{J\otimes J}{\rho}\right) + \rho\nabla f(\rho) = 0 \quad ; \quad J_{|t=0} = |a_0|^2\nabla\phi_0. \end{cases}$$

Identifying terms: $\rho = |a|^2$, $J = |a|^2\nabla\phi$.

Splitting in the semiclassical limit

Idea: as long as the solution to the exact equation writes

$$u^\varepsilon(t,x)=a^\varepsilon(t,x)e^{i\phi^\varepsilon(t,x)/\varepsilon},\quad (a^\varepsilon,\phi^\varepsilon \text{ \textit{uniformly} bounded } H^s),$$

then so does the numerical solution obtained by splitting.

ODE: $i\varepsilon\partial_t u^\varepsilon = f(|u^\varepsilon|^2)u^\varepsilon,\ u^\varepsilon_{|t=0} = a_0^\varepsilon e^{i\phi_0^\varepsilon/\varepsilon}$.

$\rightsquigarrow u^\varepsilon(t,x) = a_0^\varepsilon(x)e^{i\phi_0^\varepsilon(x)/\varepsilon - itf(|a_0^\varepsilon(x)|^2)/\varepsilon}$.

Amounts to considering the system:

$$\begin{cases} \partial_t\phi^\varepsilon = -f\left(|a^\varepsilon|^2\right) \quad ; \quad \phi^\varepsilon_{|t=0} = \phi_0^\varepsilon, \\ \partial_t a^\varepsilon = 0 \quad ; \quad a^\varepsilon_{|t=0} = a_0^\varepsilon. \end{cases}$$

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The solution can be written as $u^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$, with

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$\rightsquigarrow$ The system is *decoupled*: $\nabla\phi^\varepsilon$ solves Burgers.
Before singularity formation, solve the first equation (ϕ^ε uniformly bounded H^s), then the second is a linear PDE with bounded coefficients (a^ε uniformly bounded H^{s-2}).

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Outcome

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$\rightsquigarrow$ Generalizations: WKB regime for other equations ($f' \geqslant 0$, Schrödinger-Poisson, $f(\rho) = \lambda\rho^\sigma$).

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- The linear PDE has been replaced by a nonlinear system.
- $\nabla\phi^\varepsilon$ solves (multiD) Burgers: local resolution, propagation of H^s regularity ($s > d/2+1$), tame estimates.
- If $\nabla\phi^\varepsilon \in L^\infty([0,\tau];H^s)$, $s > d/2+1$, one cannot hope better than $a^\varepsilon \in L^\infty([0,\tau];H^{s-1})$.

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Propagating Sobolev regularity: ODE

$$\begin{cases} \partial_t \phi^\varepsilon = -f\left(|a^\varepsilon|^2\right), \\ \partial_t a^\varepsilon = 0. \end{cases}$$

- If f is local ($f(\rho) = \rho^{\gamma-1}$), then for $a^\varepsilon \in L^\infty([0,\tau]; H^\sigma)$, $\sigma > d/2$, $\phi^\varepsilon \in L^\infty([0,\tau]; H^\sigma)$ and not better: the numerical scheme does not preserve the regularity.
- The issue of loss of regularity vanishes if a Poisson type nonlinearity is considered.
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Sobolev regularity

Hypothesis

$f(\rho) = K * \rho$, where the Fourier transform of K,

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

satisfies:

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

Example

If $d \geqslant 3$, Schrödinger-Poisson: $f(|u|^2)u = V_{\rm p}u$, where $\Delta V_{\rm p} = \lambda|u|^2$, $\lambda \in \mathbb{R}$.

The exact solution

If for $s > d/2 + 1$, $\phi_0 \in L^\infty$, $(\nabla\phi_0, a_0) \in H^{s+1} \times H^s$, then there exists $T > 0$ such that the system

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

has a unique solution $(\phi^\varepsilon, a^\varepsilon) \in C([0,T]; L^\infty \times H^s)$ such that $\nabla\phi^\varepsilon \in C([0,T]; H^{s+1})$. In addition, the bounds are uniform in $\varepsilon \in]0,1]$.

We can take $T = T_{\max} - \delta$, where $T_{\max}$ is the lifespan of the Euler-Poisson system (if $T_{\max} < \infty$).

$\rightsquigarrow$ WKB form preserved for the exact solution, on $[0,T]$.

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Main result

Theorem

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* $n \in \mathbb{N}$ *such that* $t_n = n\Delta t \in [0, T]$, *we have:*

1. *There exist* ϕ^ε *and* a^ε *with*

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

such that $u^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$ *on* $[0, T] \times \mathbb{R}^d$.

2. *There exist* ϕ_n^ε *and* a_n^ε *with*

$$\|a_n^\varepsilon\|_{H^s(\mathbb{R}^d)} + \|\nabla \phi_n^\varepsilon\|_{H^{s+1}(\mathbb{R}^d)} + \|\phi_n^\varepsilon\|_{L^\infty(\mathbb{R}^d)} \leqslant C,$$

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:*

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

Back to initial unknowns

Corollary

Under the previous assumptions, with previous notations:

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

Main quadratic observables:

$$\left\| \left| (Z_\varepsilon^{\Delta t})^n u_0^\varepsilon \right|^2 - |u^\varepsilon(t_n)|^2 \right\|_{L^1(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)} \leqslant C\Delta t,$$

$$\left\| \operatorname{Im} \left(\varepsilon \overline{(Z_\varepsilon^{\Delta t})^n u_0^\varepsilon} \nabla (Z_\varepsilon^{\Delta t})^n u_0^\varepsilon \right) - J^\varepsilon(t_n) \right\|_{L^1(\mathbb{R}^d)\cap L^\infty(\mathbb{R}^d)} \leqslant C\Delta t.$$

Remark

In agreement with numerical experiments by Bao-Jin-Markowich '03.

Scheme of the proof

- Regularity estimates on the exact solution.
- (Local) regularity estimates on the numerical scheme.
- Local error estimate (after Descombes-Thalhammer).
- From local to global: Lady Windermere's fan and induction (after Holden-Lubich-Risebro).

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Analytic regularity

The phase ϕ^ε and the amplitude a^ε belong to $\mathcal{H}^\ell_\rho$, $\ell > d/2+1$, where

$$\|\psi\|^2_{\mathcal{H}^\ell_\rho} = \int_{\mathbb{R}^d} \langle\xi\rangle^{2\ell} e^{2\rho\langle\xi\rangle} |\hat{\psi}(\xi)|^2 d\xi,$$

with a time dependent weight ρ.

Inspired by the analysis of Ginibre & Velo '01. Requirements:

- $\rho(t) \geqslant \delta > 0$ on $[0, T]$,
- $-\dot{\rho}(t) \gg 1$.

For instance, $\rho(t) = M_0 - Mt$, with $M_0, M \gg 1$. Advantages:

- The previous loss of regularity issue disappears,
- No symmetry needed in the hydrodynamical form (unlike in Grenier's approach).

Typically, we can consider $f(|u|^2)u = \lambda|u|^{2\sigma}u$, $\sigma \in \mathbb{N}$, $\lambda \in \mathbb{R}$.

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Parabolization of the Euler system

The time dependent analytic norm

$$\|\psi\|^2_{\mathcal{H}^\ell_\rho} = \int_{\mathbb{R}^d} \langle\xi\rangle^{2\ell} e^{2\rho\langle\xi\rangle} |\hat{\psi}(\xi)|^2 d\xi$$

implies the general property

$$\frac{d}{dt}\|\psi\|^2_{\mathcal{H}^\ell_\rho} = 2\left\langle \partial_t\psi, \psi\right\rangle_{\mathcal{H}^\ell_\rho} + 2\dot{\rho}\|\psi\|^2_{\mathcal{H}^{\ell+1/2}_\rho}.$$

Last term: as if a parabolic term (of order 1) had been added ($\dot{\rho} < 0$).
$\rightsquigarrow$ Implicit dependence of $M = -\dot{\rho}$ in the computations: assume that the initial data a_0 and ϕ_0 satisfy

$$\int_{\mathbb{R}^d} e^{\langle\xi\rangle^{1+\delta}} \left(|\hat{a}_0(\xi)|^2 + |\hat{\phi}_0(\xi)|^2\right) d\xi < \infty,$$

for some $\delta > 0$ (e.g.: Gaussian data, or compact support on Fourier side).
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Theorem

Suppose that $d, \sigma \in \mathbb{N}$, $d, \sigma \geqslant 1$, *and* $\lambda \in \mathbb{R}$. *Let* ϕ_0, a_0 *such that*

$$\int_{\mathbb{R}^d} e^{\langle \xi \rangle^{1+\delta}} \left(|\hat{\phi}_0(\xi)|^2 + |\hat{a}_0(\xi)|^2 \right) d\xi < \infty, \text{ for some } \delta > 0.$$

$\exists T, \varepsilon_0, c_0 > 0$ *and* $(C_k)_{k \in \mathbb{N}}$ *s. t.* $\forall \varepsilon \in (0, \varepsilon_0]$, *the following holds:*
1. $\exists! u^\varepsilon = S_\varepsilon^t u_0^\varepsilon \in C([0,T], \cap_s H^s)$. *Moreover, there exist* ϕ^ε *and* a^ε *with*

$$\sup_{t \in [0,T]} \left(\|a^\varepsilon(t)\|_{H^k(\mathbb{R}^d)} + \|\phi^\varepsilon(t)\|_{H^k(\mathbb{R}^d)} \right) \leqslant C_k, \quad \forall k \in N,$$

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

$$\|a_n^\varepsilon\|_{H^k(\mathbb{R}^d)} + \|\phi_n^\varepsilon\|_{H^k(\mathbb{R}^d)} \leqslant C_k, \quad \forall k \in \mathbb{N}$$

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:*

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

Local error estimate

Let A an operator, and $\mathcal{E}_A$ its propagator:

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

Theorem (Descombes-Thalhammer)

Suppose that $F(u) = A(u) + B(u)$, and denote

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

the exact and numerical flows, respectively. The exact formula holds

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

NB: $\partial_2 \mathcal{E} =$ linearized flow.

Standard framework for NLS:

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

Linearized exact flow: $\partial_2 \mathcal{E}_F(t,u) w_0 = w$, where

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

Drawback: does not preserve the (monokinetic) WKB structure. If $u = ae^{i\phi/\varepsilon}$, then

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

For $w_0 = b_0 e^{i\varphi_0/\varepsilon}$, in general, there does not hold

$$w = b^\varepsilon e^{i\varphi^\varepsilon/\varepsilon}, \quad b^\varepsilon, \varphi^\varepsilon \text{ uniformly bounded in } H^s.$$

Remark

More simply, $a_n^\varepsilon e^{i\phi_n^\varepsilon/\varepsilon} - a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$ has no reason to be factored $\alpha_n^\varepsilon e^{i\varphi_n^\varepsilon/\varepsilon}$ (with uniform bounds).

That is another reason to work on systems:

$$\begin{cases} \partial_t \phi^\varepsilon = -f\left(|a^\varepsilon|^2\right), \\ \partial_t a^\varepsilon = 0. \end{cases}$$

and

$$\begin{cases} \partial_t \phi^\varepsilon + \frac{1}{2}|\nabla \phi^\varepsilon|^2 = 0, \\ \partial_t a^\varepsilon + \nabla \phi^\varepsilon \cdot \nabla a^\varepsilon + \frac{1}{2} a^\varepsilon \Delta \phi^\varepsilon = i\frac{\varepsilon}{2}\Delta a^\varepsilon. \end{cases}$$

Precised framework

$$A\begin{pmatrix}\phi\\ a\end{pmatrix} = \begin{pmatrix}-\frac{1}{2}|\nabla\phi|^2\\ -\nabla\phi\cdot\nabla a - \frac{1}{2}a\Delta\phi + i\frac{\varepsilon}{2}\Delta a\end{pmatrix},$$

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

Remark

Both operators are nonlinear.

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

Local error

Theorem (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*

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