On time splitting for NLS in the semiclassical limit

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Fourier time splitting methods for the nonlinear Schrödinger equation

$$i\partial_t u + \frac{1}{2}\Delta u = f\left(|u|^2\right)u, \quad t \geqslant 0,\ x \in \mathbf{R}^d, \tag{1}$$

with $u : [0,T] \times \mathbf{R}^d \to \mathbf{C}$, and $f : \mathbf{R}_+ \to \mathbf{R}$, consist in solving alternively

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

and

$$i\partial_t u = f\left(|u|^2\right)u. \tag{3}$$

Thanks to the Fourier transform, (2) is solved explicitly, and since the ordinary differential equation (3) turns out to be linear (after one has remarked that $\partial_t(|u|^2) = 0$, since f is real-valued), an explicit formula is available as well. Denoting by X^t the flow associated to (2), and by Y^t the flow associated to (3), Lie splitting method consists in considering $Z_L^{\Delta t} = Y^{\Delta t} \circ X^{\Delta t}$ or $Z_L^{\Delta t} = X^{\Delta t} \circ Y^{\Delta t}$. Higher order Fourier time splitting methods can be considered on the same basis, such as Strang splitting, $Z_S^{\Delta t} = X^{\Delta t/2} \circ Y^{\Delta t} \circ X^{\Delta t/2}$ for instance. The convergence of such methods as the time step Δt goes to zero has been established in [2] ($d \leqslant 2$) and [6] ($d = 3$). Typically, one has the following result in the cubic defocusing case $f(|u|^2)u = |u|^2 u$. For $u_0 \in H^2(\mathbf{R}^d)$ and all $T > 0$, $\exists C, h_0$ such as if $\Delta t \in]0, h_0]$, $\forall n \in \mathbf{N}$ with $n\Delta t \in [0,T]$,

$$\left\| \left(Z_L^{\Delta t}\right)^n u_0 - u(n\Delta t) \right\|_{L^2} \leqslant C\left(m_2, T\right)\Delta t, \tag{4}$$

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

In the semiclassical case

$$i\varepsilon\partial_t u^\varepsilon + \frac{\varepsilon^2}{2}\Delta u^\varepsilon = f\left(|u^\varepsilon|^2\right)u^\varepsilon, \quad \varepsilon \to 0, \tag{5}$$

considered in numerical experiments in [1], and motivated by Physics (superfluids, Bose–Einstein condensation), the above error estimate becomes irrelevant. Typically, consider WKB type initial data,

$$u^\varepsilon(0,x) = a_0(x)e^{i\phi_0(x)/\varepsilon}, \tag{6}$$

with a_0 a smooth complex-valued function, and ϕ_0 a smooth real-valued function. It is easy to see that, even in the case $\phi_0 = 0$, the scaling of (5) forces the presence of rapid oscillations in u^ε, which is ε-oscillatory. Therefore, in (4), the factor m_2 behaves like ε^{-2} as $\varepsilon \to 0$, and (4) becomes rather unsatisfactory. To overcome this issue, the idea is that the splitting scheme preserves the WKB form (6), in the following sense: at least for some time, the numerical solution, at time $t_n = n\Delta t$, is of the form

$$u_n^\varepsilon(x) = a_n^\varepsilon(x)e^{i\phi_n^\varepsilon/\varepsilon}, \tag{7}$$

where a_n^ε and ϕ_n^ε must be expected to depend on ε, but remain bounded in Sobolev spaces *uniformly in* $\varepsilon \in (0,1]$. A similar property holds for the exact solution u^ε: seeking $u^\varepsilon = a^\varepsilon e^{i\phi^\varepsilon/\varepsilon}$, one is led to considering the system

$$
\begin{cases} \partial_t \phi^\varepsilon + \dfrac{1}{2}|\nabla\phi^\varepsilon|^2 = -f\left(|a^\varepsilon|^2\right), \\ \partial_t a^\varepsilon + \nabla\phi^\varepsilon\cdot\nabla a^\varepsilon + \dfrac{1}{2}a^\varepsilon\Delta\phi^\varepsilon = i\dfrac{\varepsilon}{2}\Delta a^\varepsilon. \end{cases} \tag{8}
$$

Letting $\varepsilon = 0$ in (8), and considering $(v = \nabla\phi, a)$ as a new unknown, one recovers the compressible Euler equation with pressure law related to f, in its symmetric form. For that reason, we must consider time for which the solution to

$$
\begin{cases} \partial_t v + v\cdot\nabla v + \nabla f\left(\rho\right), \quad v_{|t=0} = \nabla\phi_0, \\ \partial_t \rho + \operatorname{div}(\rho v) = 0, \quad \rho_{|t=0} = |a_0|^2, \end{cases} \tag{9}
$$

remains smooth. Then the time splitting scheme applied to (5) preserves the form (7), and amounts to doing time splitting on (8). Unfortunately, by this remark, we see that one has to face a loss of regularity issue, which brings us to make the following assumption:

Assumption 1. *The nonlinearity f is of the form $f(\rho) = K * \rho$, where the kernel K is such that its Fourier transform 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 $\lambda \in \mathbf{R}$. Our main result is he following.

Theorem 2. *Suppose that $d \geqslant 1$, and that f satisfies Assumption 1. 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 (9) satisfies $(v, \rho) \in C([0,T]; H^{s+1}\times H^s)$. Consider $u^\varepsilon = S_\varepsilon^t u_0^\varepsilon$ solution to (5) and u_0^ε given by (6). 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_n^ε and a_n^ε with*

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

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:*

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

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. Also, this result shows that it is possible to approximate the wave function u^ε provided that $\Delta t = o(\varepsilon)$, and to approximate quadratic observables provided that $\Delta t = o(1)$: the time step can be chosen independent of $\varepsilon \in (0, 1]$, which agrees with the numerical observations made in [1].

The proof of this result then relies on a general strategy used in [5], a general local error formula for Lie splitting scheme derived in [4], and on various estimates. The details are available in [3].

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References

[1] W. Bao, S. Jin, and P. A. Markowich, *Numerical study of time-splitting spectral discretizations of nonlinear Schrödinger equations in the semiclassical regimes*, SIAM J. Sci. Comput. **25** (2003), no. 1, 27–64.

[2] 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), no. 1, 26–40.

[3] R. Carles, *On Fourier time-splitting methods for nonlinear Schrödinger equations in the semi-classical limit*, SIAM J. Numer. Anal., to appear.

[4] S. Descombes and M. Thalhammer, *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), no. 2, 722–745.

[5] H. Holden, C. Lubich, and N. H. Risebro, *Operator splitting for partial differential equations with Burgers nonlinearity*, Math. Comp. **82** (2013), no. 281, 173–185.

[6] C. Lubich, *On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations*, Math. Comp. **77** (2008), no. 264, 2141–2153.