Analysis of a relaxation scheme for a nonlinear Schrödinger equation occurring in Plasma Physics

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Abstract. This paper is devoted to the analysis of a relaxation-type numerical scheme for a nonlinear Schrödinger equation arising in plasma physics. The scheme is shown to be preservative in the sense that it preserves mass and energy. We prove the well-posedness of the semidiscretized system and prove convergence to the solution of the time-continuous model.

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1 Introduction

The design of numerical schemes for nonlinear Schrödinger equations and the convergence analysis have been a very active field since decades. Such an interest is justified by the various applications of the Schrödinger equation in several fields. The basic schemes are of Crank-Nicholson, Runge-Kutta, symplectic and splitting types [1, 10, 2, 7, 11, 12, 13, 14, 8] and most of those schemes have the main drawback of being nonconservative. In general they do not conserve the total energy while most of the continuous models do, except in some special situations when dissipation or gain of the energy occurs. Also, these models suffer from oscillations in the semi-classical regime if the time and space steps are not very small and we refer to [9] for further references and a rich review article on the topic.

The aim of this paper is the formulation and the analysis of a relaxation scheme for the following nonlinear Schrödinger equation arising in plasma physics,

$$\mathcal{S}_c : \quad \begin{cases} i\partial_t u = -\Delta u - \operatorname{div}\left(|\nabla\phi|^2 \nabla\phi\right) , \quad t \geq 0 , \quad x \in \mathbb{R}^3 , \\ \Delta\phi = u , \quad u(t=0,x) = u_0(x) . \end{cases}$$

The operator $\Delta = \nabla^2$ denotes the laplacian, ∂_t the partial derivative with respect to time and div denotes the divergence operator.

In the framework of long wave oscillations, the low frequency motions in a nonlinear plasma can be considered quasi-neutral. The linearized hydrodynamical equations for an electron gaz and Maxwell's equations offer then a possible mathematical description (neglecting the interaction of high frequency oscillations) for the evolution of the electric field E

$$(\partial_t^2 + \omega_e^2)\, E + c^2\, \nabla \wedge (\nabla \wedge E) - 3v_{T_e}^2 \nabla \mathrm{div} E + \omega_e^2\, \frac{\delta_n}{n_0}\, E = 0,$$

where ∂_t^2 denotes the second partial derivative with respect to time and $\nabla \wedge \cdot$ denotes the rotational operator. Also, ω_e, n_0 and v_{T_e} denote the pulsation of the plasma, the density of electrons and the thermal electron velocity respectively. Now, we assume that the frequency of the oscillations is close to that of the plasma and let $E = e^{i\omega_p t}\, \tilde{E}$ with $\partial_t \tilde{E} << \omega_p\, \tilde{E}$. Furthermore, if we neglect the second time derivative term and assume that the electron distribution follows the Bolzmann's law $\frac{\delta_n}{n_0} = \frac{|\tilde{E}|^2}{16\pi n_0 (T_e + T_i)}$ where T_e and T_i denote the electron and ion temperatures respectively, the PDE above becomes

$$2i\omega_p \partial_t \tilde{E} + c^2\, \nabla \wedge (\nabla \wedge \tilde{E}) - 3v_{T_e}^2 \nabla \mathrm{div} \tilde{E} + \frac{\omega_p^2}{16\pi n_0 (T_e + T_i)} |\tilde{E}|^2\, \tilde{E} = 0.$$

In the potential case, we have $\tilde{E} = \nabla\phi$, therefore, if we apply the div operator on both sides of the PDE above and use a scaling argument, we obtain the system $\mathcal{S}_c$ and we refer the reader to [3] for more details concerning the formal derivation of this family of models.

The system $\mathcal{S}_c$ has been formally derived and analyzed in [5]. In particular it is shown that it enjoys the following conservation laws

$$\begin{aligned} &\mathcal{N}(t) = \int_{\mathbb{R}^3} |\nabla\phi(t,x)|^2 dx = \mathcal{N}(t=0)\ , \\ &\mathcal{E}(t) = \frac{1}{2}\int_{\mathbb{R}^3} |\Delta\phi(t,x)|^2 dx - \frac{1}{4}\int_{\mathbb{R}^3} |\nabla\phi(t,x)|^4 dx = \mathcal{E}(t=0)\ . \end{aligned} \tag{1.1}$$

Let $H^k(\mathbb{R}^3)$ denote the usual Sobolev space of order $k = 1, 2, ...$ and let us introduce the space

$$\mathcal{H}^k = \left\{ f \in L^6(\mathbb{R}^3) \cap C(\mathbb{R}^3) :\ \nabla f \in H^k(\mathbb{R}^3) \right\}\ ,$$

endowed with the norm $\|f\|_{\mathcal{H}^k} = \|\nabla f\|_{H^k}$. For the mathematical analysis of the system $\mathcal{S}_c$, we study the following system

$$\mathcal{S}_c' : \quad \begin{cases} i\partial_t \nabla\phi = -\Delta\nabla\phi + \nabla(-\Delta^{-1})\, \mathrm{div}\left(|\nabla\phi|^2\, \nabla\phi\right), \\ \Delta\phi = u, \quad \phi(t=0,x) = \phi_0(x). \end{cases}$$

Let us summarize the properties of the operator $\nabla(-\Delta^{-1})\,\mathrm{div}$. For that purpose, we introduce the following space

$$\mathcal{V} := \left\{ f \in (\mathcal{D}'(\mathbb{R}^3))^3 \quad \text{such that} \quad \exists\phi \in \mathcal{D}'(\mathbb{R}^3) \quad \text{with} \quad \nabla\phi = f \right\}.$$

In Ref. [5], it is proved that there exists an operator $\mathbf{B}$ continuous on $L^p(\mathbb{R}^3)$ for all $1 < p < \infty$ such that its restriction to functions in $\mathcal{D}(\mathbb{R}^3)$ coincides with the operator $\nabla(-\Delta^{-1})\,\mathrm{div}$. In particular, for all $f \in L^p(\mathbb{R}^3)$ ($1 < p < \infty$), one has $\mathrm{div}\,\mathbf{B}\,f = \mathrm{div}\,f$, $\mathbf{B}\,f \in \mathcal{V}$ and $\|\mathbf{B}\,f\|_{L^p} \le c\,\|f\|_{L^p}$, where c is a universal constant. It is also proved that there exists an operator $\mathbf{C}$ such that if $f \in \mathcal{D}(\mathbb{R}^3)$, then $\mathbf{C}$ coincides with $\nabla(-\Delta)^{-1}$ and maps continuously $L^p(\mathbb{R}^3)$ into $L^{\frac{3p}{3-p}}$ for all $1 < p < 3$. Moreover, if $\mathrm{div}f \in L^p(\mathbb{R}^3)$ and $f \in L^{\frac{3p}{3-p}}$ then $\mathbf{C}(\mathrm{div}f) = \mathbf{B}\,f$ for all $1 < p < 3$. Therefore, the property $\nabla(-\Delta)^{-1}\mathrm{div}f = \mathbf{B}f$ holds true on $\mathcal{D}(\mathbb{R}^3)$ and by density for regular enough functions. With this definition in mind, it is rather easy to show that the systems $\mathcal{S}_c$ and $\mathcal{S}_c'$ are equivalent as soon as $\phi \in C([0,T],\mathcal{H}^1)$ (cf. [5]). Next, one introduces the functional

$$\mathcal{T} : \nabla\phi \mapsto e^{it\Delta}\nabla\phi_0 - i\int_0^t e^{i(t-s)\Delta}\nabla(-\Delta^{-1})\,\mathrm{div}\left(|\nabla\phi(s)|^2\,\nabla\phi(s)\right)\,ds\ ,$$

where $e^{it\Delta}$ denotes the group generated by the free Schrödinger equation $i\partial_t u = -\Delta\,u$. It is rather standard to prove that $\phi \in L^\infty([0,T],\mathcal{H}^1)$ satisfies $\mathcal{T}(\nabla\phi) = \nabla\phi$ if and only if ϕ satisfies $\mathcal{S}_c'$ (equivalently $\mathcal{S}_c$) (cf. [5]). Next, we introduce the following functional spaces

$$\begin{aligned} X &:= \left\{\nabla f \in L^\infty([0,T],L^2(\mathbb{R}^3)\cap\mathcal{V})\cap L^{\frac{8}{3}}([0,T],L^4(\mathbb{R}^3)\cap\mathcal{V})\right\}, \\ Y &:= \left\{\nabla f \in X,\ \nabla^2 f \in L^\infty([0,T],L^2(\mathbb{R}^3))\cap L^{\frac{8}{3}}([0,T],L^4(\mathbb{R}^3))\right\} \subset X\ . \end{aligned}$$

In Ref. [5], using Strichartz estimates, the author shows that for large enough radius R, the mapping $\mathcal{T}$ maps the ball of a well chosen radius R in Y into itself and is a contraction in the X norm for small enough time $T > 0$. Thus there exists a unique solution $\nabla\phi \in C([0,T],H^1)$ to the equation

$$i\partial_t\nabla\phi = -\Delta\nabla\phi + \nabla(-\Delta^{-1})\,\mathrm{div}\left(|\nabla\phi|^2\,\nabla\phi\right).$$

Since $X \subset \mathcal{V}$, it holds that $\nabla\phi$ is the gradient of $\phi \in \mathcal{D}'$. Eventually, thanks to the fact that $\{f \in H^1(\mathbb{R}^3)^3,\ \exists\phi \in \mathcal{D}',\ \nabla\phi = f\} = \{\nabla\phi,\ \phi \in \mathcal{H}^1\}$, we can choose $\phi \in \mathcal{H}^1$. The global-in-time existence is obtained using the conservation laws with a smallness assumption on the initial data.

In summary, we have the following

Theorem 1 [[5]]. *Let $\phi_0 \in \mathcal{H}^1$, then there exists a positive time $T(\phi_0) > 0$ such that the system*

$$\begin{cases} i\partial_t\nabla\phi = -\Delta\nabla\phi + \nabla(-\Delta^{-1})\,\mathrm{div}\left(|\nabla\phi|^2\,\nabla\phi\right)\ , \\ \phi(t=0,x) = \phi_0(x)\ . \end{cases} \tag{1.2}$$

admits a unique maximal solution $\phi \in C^0([0,T(\phi_0)[,\mathcal{H}^1)$. In particular, ϕ is the unique solution to $\mathcal{S}_c$. Moreover, if $\|\phi_0\|_{\mathcal{H}^1}$ is small enough, then $T(\phi_0) = +\infty$.

It is rather easy to extend Theorem 1 as follows

Corollary 1. Let $\phi_0 \in \mathcal{H}^m$, $m \geq 1$, then the unique solution ϕ according to Theorem 1 is in fact in $C^0([0,T(\phi_0)[,\mathcal{H}^m)$. Moreover, the following regularity holds

$$\phi \in C^0([0,T(\phi_0)[,\mathcal{H}^m) \,\cap\, C^1([0,T(\phi_0)[,\mathcal{H}^{m-2}) \,\cap\, C^2([0,T(\phi_0)[,\mathcal{H}^{m-4}).$$

Proof. The first claim of the Theorem is easy and we refer to [5]. Let us sketch the proof of the regularity part. We have obviously following the first part that $\nabla\phi \in C^0([0,T(\phi_0)[,H^m)$. Therefore

$$\partial_t \nabla\phi = i\Delta\nabla\phi - i\nabla(-\Delta^{-1})\,\mathrm{div}\left(|\nabla\phi|^2\,\nabla\phi\right) \in C^0([0,T(\phi_0)[,H^{m-2}).$$

The loss of regularity is due to the Laplacian. Now, we set $\boldsymbol{\psi} = \partial_t\nabla\phi$ and observe that the formal derivative with respect to time of (1.2) implies that

$$\partial_t\boldsymbol{\psi} = i\Delta\boldsymbol{\psi} - i\nabla\,(-\Delta^{-1})\,\mathrm{div}\,(2\,\Re(\boldsymbol{\psi}\nabla\bar{\phi})\,\nabla\phi + |\nabla\phi|^2\boldsymbol{\psi}).$$

Hence it holds easily that $\partial_t\boldsymbol{\psi} = \partial_t^{(2)}\nabla\phi \in C^0([0,T(\phi_0)[,H^{m-4})$, which finishes the proof.

Now, we turn to the discretization in time of our problem. As pointed above, the systems $\mathcal{S}_c$ and $\mathcal{S}'_c$ being equivalent, we shall focus on the former one. The discretization in space can be achieved with finite differences or finite elements methods. We consider N points for the time discretization so that for the computation time it holds that $T_{\delta t} < T$ where T is the existence time of the solution of the continuous system. The time step δt is given by $\delta t = \frac{T_{\delta t}}{N}$. We shall denote by f^n the approximation of the continuous function f at time $t_n = n\delta t$. Eventually, we define $f_{\delta t}(t,x) = \sum_{n=0}^{N-1} f^n(x)\mathbf{I}_{[t_n,t_{n+1})}(t)$ where $\mathbf{I}_{[t_n,t_{n+1})}$ is the characteristic function on the half open interval $[t_n,t_{n+1})$. Now, in order to construct a conservative scheme, we follow the relaxation method of Besse developed in [4] for the case of a Schrödinger equation with an even integer power nonlinearity. For that purpose, we introduce an extra variable ξ to the system $\mathcal{S}'_c$ as follows

$$\begin{cases} i\partial_t\nabla\phi = -\Delta\nabla\phi + \nabla(-\Delta^{-1})\,\mathrm{div}\,(\xi\,\nabla\phi)\ , \\ \xi = |\nabla\phi|^2\ , \\ \phi(t=0,x) = \phi_0(x)\ , \end{cases} \tag{1.3}$$

where we have omitted $u = \Delta\phi$, as this quantity can be computed in a post-processing step. Next, we consider its discretized version at times $t_n = n\,\delta t$ and $t_{n+\frac{1}{2}} = (n+\frac{1}{2})\,\delta t$ that reads as follows

$$\mathcal{S}_d : \begin{cases} i\dfrac{\nabla\phi^{n+1} - \nabla\phi^n}{\delta t} = -\Delta\dfrac{\nabla\phi^{n+1} + \nabla\phi^n}{2} + \\ \qquad\qquad + \nabla(-\Delta^{-1})\,\mathrm{div}\left(\xi^{n+\frac{1}{2}}\,\dfrac{\nabla\phi^{n+1} + \nabla\phi^n}{2}\right), \\ \dfrac{\xi^{n+\frac{1}{2}} + \xi^{n-\frac{1}{2}}}{2} = |\nabla\phi^n|^2\ , \\ \phi(t=0,x) = \phi_0(x)\ , \quad \xi^{-\frac{1}{2}} = |\nabla\phi_0|^2\ . \end{cases}$$

First we show the existence of a solution to the semi-discrete scheme, i.e.

Theorem 2. *Let $\phi_0 \in \mathcal{H}^m$ with $m > \frac{3}{2}$, then there exists a unique maximal solution $(\phi_{\delta t}, \xi_{\delta t})$ of $\mathcal{S}_d$ in $L^\infty([0, T_{\delta t}]; \mathcal{H}^m \times H^m)$ such that*

$$\sup_{t \in [0, T_{\delta t}]} \left(\|\phi_{\delta t}\|_{\mathcal{H}^m} + \|\xi_{\delta t}\|_{H^m} \right) \leq C(T, \|\phi_0\|_{\mathcal{H}^m}) \ .$$

Furthermore we prove the convergence to the continuous solution according to Theorem 1 and Corollary 1.

Theorem 3. *Let $\phi_0 \in \mathcal{H}^{m+4}$ and ϕ be the maximal solution of $\mathcal{S}_c$ according to Theorem 1 and Corollary 1, then it holds that* $\liminf_{\delta t \to 0} T_{\delta t} \geq T$ *and $\forall \tau < T$, the solution $(\phi_{\delta t}, \xi_{\delta t})$ to $\mathcal{S}_d$ converges to $(\phi, |\nabla \phi|^2)$ as $\delta_t \to 0$ in $L^\infty([0, \tau]; \mathcal{H}^m \times H^m)$.*

The outline of the paper is as follows. In Section 2 we prove that the scheme $\mathcal{S}_d$ conserves discretized versions of the quantities defined in (1.1). In Section 3 we prove Theorem 2, i.e. the existence of a unique maximal solution to the scheme $\mathcal{S}_d$. In Section 4 we prove the convergence of these discretized solutions to the solution of $\mathcal{S}_c'$ according to Theorem 1 which we have formulated in Theorem 3.

2 Conservation Laws

In this section, we show that our scheme conserves the physical quantities *mass* and *energy*. These properties guarantee some stability of numerical simulations. Indeed, we claim that the discrete system $\mathcal{S}_d$ enjoys the following property.

Lemma 1. *Assume that $\mathcal{S}_d$ admits a solution $(\phi^n, \xi^{n+\frac{1}{2}})_n$ in $\ell^\infty([0, N]; \mathcal{H}^2 \times H^2)$. Then*

$$\int_{\mathbb{R}^3} |\nabla \phi^N|^2 \, dx = \int_{\mathbb{R}^3} |\nabla \phi_0|^2 \, dx \ . \tag{2.1}$$

$$\int_{\mathbb{R}^3} \left(|\Delta \phi^N|^2 - \frac{1}{2} \xi^{N+\frac{1}{2}} \xi^{N-\frac{1}{2}} \right) dx = \int_{\mathbb{R}^3} \left(|\Delta \phi_0|^2 - \frac{1}{2} \xi^{\frac{1}{2}} \xi^{-\frac{1}{2}} \right) dx \ . \tag{2.2}$$

Proof. The proof is based on formal calculation that can be made rigorous using standard regularization arguments. On the one hand, we multiply the first line of $\mathcal{S}_d$ by $\nabla \bar{\phi}^{n+1} + \nabla \bar{\phi}^n$ and integrate over $\mathbb{R}^3$. Using an integration by parts, one obtains

$$\begin{aligned}
\frac{i}{\delta t} \int_{\mathbb{R}^3} & |\nabla \phi^{n+1}|^2 - |\nabla \phi^n|^2 dx = \\
&= \int_{\mathbb{R}^3} \frac{1}{2} \left(\left| \Delta(\phi^{n+1} + \phi^n) \right|^2 - \frac{2}{\delta t} \Im \left(\nabla \phi^n \nabla \bar{\phi}^{n+1} \right) \right) dx - \\
&\quad - \frac{1}{2} \int_{\mathbb{R}^3} \Delta(-\Delta^{-1}) \mathrm{div} \left(\xi^{n+\frac{1}{2}} \, \nabla(\phi^{n+1} + \phi^n) \right) (\bar{\phi}^{n+1} + \bar{\phi}^n) \, dx \ .
\end{aligned}$$

Taking the imaginary part, we get

$$\frac{1}{\delta t} \int_{\mathbb{R}^3} |\nabla \phi^{n+1}|^2 - |\nabla \phi^n|^2 dx = -\frac{1}{2} \Im \int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}} \, |\nabla(\phi^{n+1} + \phi^n)|^2 \, dx \ .$$

Now, from the second equation of the system $\mathcal{S}_d$ we conclude that $\xi^{n+\frac{1}{2}}$ can be computed as a real valued linear combination of $|\nabla\phi^k|$, $k = 0...n$. Therefore, we have that $-\frac{1}{2}\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}} \, |\nabla(\phi^{n+1} + \phi^n)|^2 \, dx$ is real valued and we get $\int_{\mathbb{R}^3} |\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2 dx = 0$. Eventually, a summation with respect to n proves (2.1).

On the other hand, in order to prove (2.2) we proceed in two steps. The first step consists in multiplying the second equation of $\mathcal{S}_d$ by $\xi^{n+\frac{1}{2}} - \xi^{n-\frac{1}{2}}$, thus getting

$$\left(\xi^{n+\frac{1}{2}}\right)^2 - \left(\xi^{n-\frac{1}{2}}\right)^2 = 2|\nabla\phi^n|^2 \left(\xi^{n+\frac{1}{2}} - \xi^{n-\frac{1}{2}}\right).$$

Therefore, a summation over n gives

$$\begin{aligned}\left(\xi^{N-\frac{1}{2}}\right)^2 - \left(\xi^{-\frac{1}{2}}\right)^2 &= -2\sum_{n=0}^{N-1} \left(|\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2\right) \xi^{n+\frac{1}{2}} \\ &- 2|\nabla\phi^0|^2\xi^{-\frac{1}{2}} + 2|\nabla\phi^N|^2\xi^{N-\frac{1}{2}}.\end{aligned} \tag{2.3}$$

The second step consists in multiplying the first line of $\mathcal{S}_d$ by $\nabla\bar{\phi}^{n+1} - \nabla\bar{\phi}^n$ and integrating over $\mathbb{R}^3$. Therefore, after an integration by parts, one obtains

$$\begin{aligned}\frac{i}{\delta t}\int_{\mathbb{R}^3} |\nabla\left(\phi^{n+1} - \phi^n\right)|^2 dx &= +\frac{1}{2}\int_{\mathbb{R}^3} \left(|\Delta\phi^{n+1}|^2 - |\Delta\phi^n|^2\right) dx \\ - \quad \frac{1}{2}\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}} &\left(|\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2\right) dx + i\Im\int_{\mathbb{R}^3} \Delta\phi^n\Delta\bar{\phi}^{n+1}dx \\ - \quad i\Im\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}}\nabla\phi^n\nabla\bar{\phi}^{n+1} \, dx \, .\end{aligned}$$

Taking the real part of the above equality, we get

$$\frac{1}{2}\int_{\mathbb{R}^3} \left(|\Delta\phi^{n+1}|^2 - |\Delta\phi^n|^2\right) dx - \frac{1}{2}\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}} \left(|\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2\right) dx = 0 \, .$$

Therefore, summing over n leads to

$$\int_{\mathbb{R}^3} \left(|\Delta\phi^N|^2 - |\Delta\phi_0|^2\right) dx = +\sum_{n=0}^{N-1}\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}} \left(|\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2\right) dx \, .$$

Hence with (2.3), we obtain

$$\begin{aligned}\int_{\mathbb{R}^3} &\left[|\Delta\phi^N|^2 - |\nabla\phi^N|^2\xi^{N-\frac{1}{2}} + \frac{1}{2}\left(\xi^{N-\frac{1}{2}}\right)^2\right] dx \\ &= \int_{\mathbb{R}^3} \left[|\Delta\phi^0|^2 - |\nabla\phi_0|^2\xi^{-\frac{1}{2}} + \frac{1}{2}\left(\xi^{-\frac{1}{2}}\right)^2\right] dx \, .\end{aligned}$$

Eventually, multiplying the second equation of the system $\mathcal{S}_d$ by $\xi^{n-\frac{1}{2}}$ and integrating one gets

$$\frac{1}{2}\int_{\mathbb{R}^3} \xi^{n+\frac{1}{2}}\xi^{n-\frac{1}{2}}dx = \int_{\mathbb{R}^3} \left(|\nabla\phi^n|^2\xi^{n-\frac{1}{2}} - \frac{1}{2}\left(\xi^{n-\frac{1}{2}}\right)^2\right) dx \, .$$

This shows (2.2) and finishes the proof.

3 Local existence

In this section we shall prove the existence and uniqueness of local-in-time solutions to the system $\mathcal{S}_d$. Our argument is based on a classical Fixed Point Theorem application. First of all we need the following obvious fact, which is a generalization of Lemma 4 in [5], which we already cited in the introduction.

Lemma 2. *The operator* $\nabla(-\Delta^{-1})\,\mathrm{div}$ *is continuous on every* H^m *for all* $m \geq 1$.

Proof. If $f \in \mathcal{D}(\mathbb{R}^3)$, we define the operator $\mathbf{B} = (-\Delta)^{-1}\mathrm{div} f$ by

$$(-\Delta)^{-1}\mathrm{div} f = c \int \frac{(\mathrm{div} f)(y)}{|x-y|}\, dy \ ,$$

where c is a universal constant. Now, for all $1 \leq i \leq 3$ we have $\frac{d}{dx_i}\nabla(-\Delta)^{-1}\mathrm{div} f = \nabla(-\Delta)^{-1}\mathrm{div} f_{x_i}$. Thanks to the Calderón-Zygmund theorem, since $\nabla(-\Delta)^{-1}\mathrm{div}$ is homogeneous of order zero in Fourier variable, there is $C_i > 0$ such that $\|\frac{d}{dx_i}(\mathbf{B}f)\|_{L^2} = \|\mathbf{B}f_{x_i}\|_{L^2} \leq C_i \|f_{x_i}\|_{L^2}$. By iterating this argumentation we obtain that for given $m \in \mathbb{N}$, there is $C > 0$ such that

$$\|\mathbf{B}f\|_{H^m} \leq C\|f\|_{H^m}$$

for all $f \in \mathcal{D}(\mathbb{R}^3)$. We can now extend $\mathbf{B}$ to H^m by continuity.

As pointed out in [4], trying to express $\xi^{n+\frac{1}{2}}$ in terms of $|\nabla\phi^n|^2$ and substituting it in the first equation of the system leads to a loss of uniformity with respect to time. The reason is that the second equality in $\mathcal{S}_d$ implies $\xi^{N+\frac{1}{2}} = |\nabla\phi^0|^2 + 2\sum_{k=1}^{N/2} \delta t \frac{|\nabla\phi^{2k}|^2 - |\nabla\phi^{2k-1}|^2}{\delta t}$ for even N and a similar expression for odd N, which is a disretization of $\xi(T,x) = |\nabla\phi_0(x)|^2 + 2\int_0^T \partial_t |\nabla\phi|^2\, dt$. Therefore, we have to discard this idea. Also, if one considers $\mathcal{S}_d$ as a system describing the evolution of two variables ϕ and ξ, then intuitively one applies a contraction argument to the associated Duhamel formula as a functional on H^m spaces. However, in order to achieve this, one has to obtain a discrete evolution equation for ξ. A simple calculation gives $\frac{\xi^{n+\frac{1}{2}} - \xi^{n-\frac{3}{2}}}{2\delta t} = \frac{|\nabla\phi^n|^2 - |\nabla\phi^{n-1}|^2}{\delta t}$ and the first equation in $\mathcal{S}_d$ implies that

$$\frac{1}{\delta t}\left(|\nabla\phi^{n+1}|^2 - |\nabla\phi^n|^2\right) = -\frac{1}{2}\Im\left(\Delta\left(\nabla\phi^{n+1} + \nabla\phi^n\right)\nabla\left(\overline{\phi^{n+1}} + \overline{\phi^n}\right)\right) + \dots$$

Clearly, a loss of regularity occurs because of the Laplace operator appearing on the right hand side of the equation.

The retained strategy consists in introducing an extra variable into the system. Indeed, we let $\boldsymbol{\psi} = \partial_t\nabla\phi$ and the system (1.3) is now recasted as follows

$$\tilde{\mathcal{S}}_c : \quad \begin{cases} i\partial_t\nabla\phi = -\Delta\nabla\phi + \nabla\left(-\Delta^{-1}\right)\mathrm{div}\left(\Phi\right) \ , \\ \partial_t\xi = \Xi \ , \\ i\partial_t\boldsymbol{\psi} = -\Delta\boldsymbol{\psi} + \nabla\left(-\Delta^{-1}\right)\mathrm{div}\left(\Psi\right) \ . \end{cases}$$

where

$$\Phi := \xi \nabla\phi \,, \quad \Xi := 2\,\Re\left(\boldsymbol{\psi}\nabla\bar{\phi}\right) \quad \text{and} \quad \Psi := 2\,\Re(\boldsymbol{\psi}\nabla\bar{\phi})\,\nabla\phi + \xi\,\boldsymbol{\psi}\,.$$

Now, we consider the forward discretization for $\boldsymbol{\psi}$, $\boldsymbol{\psi}^{n+\frac{1}{2}} = \frac{\nabla\phi^{n+1}-\nabla\phi^{n}}{\delta t}$. Starting with $\mathcal{S}_d$ we obtain after some calculation the discretized version of $\tilde{\mathcal{S}}_c$,

$$\tilde{\mathcal{S}}_d : \begin{cases} i\dfrac{\nabla\phi^{n+2}-\nabla\phi^{n+1}}{\delta t} = -\Delta\dfrac{\nabla\phi^{n+2}+\nabla\phi^{n+1}}{2} + \nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Phi^{n+\frac{3}{2}}\right), \\ \dfrac{\xi^{n+\frac{3}{2}}-\xi^{n-\frac{1}{2}}}{2\delta t} = \Xi^{n+\frac{1}{2}}\,, \\ i\dfrac{\boldsymbol{\psi}^{n+\frac{3}{2}}-\boldsymbol{\psi}^{n-\frac{1}{2}}}{2\delta t} = -\Delta\dfrac{\boldsymbol{\psi}^{n+\frac{3}{2}}+2\boldsymbol{\psi}^{n+\frac{1}{2}}+\boldsymbol{\psi}^{n-\frac{1}{2}}}{4} \\ \qquad\qquad\qquad\qquad + \nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Psi^{n+\frac{1}{2}}\right)\,, \end{cases}$$

where

$$\begin{aligned} \Phi^{n+\frac{3}{2}} &= \xi^{n+\frac{3}{2}}\,\frac{\nabla\phi^{n+2}+\nabla\phi^{n+1}}{2}\,, \\ \Xi^{n+\frac{1}{2}} &= 2\Re\left(\boldsymbol{\psi}^{n+\frac{1}{2}}\,\frac{\nabla\bar{\phi}^{n+1}+\nabla\bar{\phi}^{n}}{2}\right)\,, \\ \Psi^{n+\frac{1}{2}} &= 2\Re\left(\boldsymbol{\psi}^{n+\frac{1}{2}}\,\frac{\nabla\bar{\phi}^{n+1}+\nabla\bar{\phi}^{n}}{2}\right)\frac{\nabla\phi^{n+2}+\nabla\phi^{n+1}+\nabla\phi^{n}+\nabla\phi^{n-1}}{4} \\ &\quad + \frac{\xi^{n+\frac{3}{2}}+\xi^{n-\frac{1}{2}}}{2}\,\frac{\boldsymbol{\psi}^{n+\frac{3}{2}}+2\boldsymbol{\psi}^{n+\frac{1}{2}}+\boldsymbol{\psi}^{n-\frac{1}{2}}}{4}\,. \end{aligned} \tag{3.1}$$

From now on, we shall use the notation $U(t) = \exp(it\Delta)$ for the free Schrödinger propagator. It is well known that $U(t)$ defines a unitary operator on the Sobolev spaces H^m. Let the operators A, B and $\mathcal{X}$ such that $A = \left(1-\frac{i}{2}\delta t\Delta\right)^{-1}, B = A\left(1+\frac{i}{2}\delta t\Delta\right)$ and $\mathcal{X}^k = (1+B)^{-1}(B^k-(-1)^k)$. Also, it is well known that A and $A\mathcal{X}^k$ are bounded operators on the Sobolev spaces H^m with bounds less than one, thereby in $\mathcal{H}^m$. Eventually, let $U_{\delta t}(t) = \sum_{n=0}^{N-1} B^n \mathbf{I}_{[n\delta t,(n+1)\delta t[}$. Moreover $A \xrightarrow[\delta t\to 0]{} 1$ and $\mathcal{U}_{\delta t}(t) \xrightarrow[\delta t\to 0]{} U(t)$ for the strong topology of operators. We summarize these facts in the following preliminary Lemma and refer to any textbook of numerical analysis for a proof

Lemma 3.

1. *A is a bounded operator on H^m for all $m \geq 1$ and $\|A\| \leq 1$.*
2. *B is a unitary operator on H^m for all $m \geq 1$.*
3. *$A\mathcal{X}^k$ is a bounded operator on H^m for all $m \geq 1$ and $\|A\mathcal{X}^k\| \leq 1$.*
4. *$\lim_{\delta t\to 0} U_{\delta t}(t) = U(t)$ for the strong topology of operators.*

5. $\lim_{\delta t\to 0} B = 1$.

Eventually, we define the following set of initial data

$$\xi^{-\frac{1}{2}} = \xi^{\frac{1}{2}} = |\nabla\phi^0|^2 \qquad \boldsymbol{\psi}^{-\frac{1}{2}} = \tfrac{1}{\delta t}(\nabla\phi^0 - \nabla\phi^{-1})\,,$$

$$\boldsymbol{\psi}^{\frac{1}{2}} = \tfrac{1}{\delta t}(\nabla\phi^1 - \nabla\phi^0) \quad \nabla\phi^0 = \nabla\phi_0\,.$$

and ϕ^{-1} such that

$$B\nabla\phi^{-1} = (B+1)\nabla\phi^0 - \nabla\phi^1\,. \tag{3.2}$$

This definition is motivated by the fact that as a consequence it holds that

$$\mathcal{X}^{n+2}\boldsymbol{\psi}^{\frac{1}{2}} + \mathcal{X}^{n+1}B\boldsymbol{\psi}^{-\frac{1}{2}} = B^{n+2}\boldsymbol{\psi}^{-\frac{1}{2}}\,. \tag{3.3}$$

As this expression appears in the Duhamel formulation of $\tilde{\mathcal{S}}_d$ this property will contribute to guaranteeing that the integral formulation of the solution operator to $\tilde{\mathcal{S}}_d$ is bounded in a suitable H^m space.

In order to prove the existence and uniqueness of solutions to this system we shall proceed in several steps. First of all, we prove that the systems $\mathcal{S}_d$ and $\tilde{\mathcal{S}}_d$ are equivalent. For that purpose, assume that $(\nabla\phi^{n+1}, \xi^{n+\frac{1}{2}}, \boldsymbol{\psi}^{n+\frac{1}{2}})$ is a solution to $\tilde{\mathcal{S}}_d$. We have only to prove that $\boldsymbol{\psi}^{n+\frac{1}{2}} = \delta t^{-1}(\nabla\phi^{n+1} - \nabla\phi^n)$ and $\xi^{n+\frac{1}{2}} + \xi^{n-\frac{1}{2}} = 2\,|\nabla\phi^n|^2$ since by construction $(\nabla\phi^{n+1}, \xi^{n+\frac{1}{2}})$ is a solution at $t = (n+\frac{1}{2})\,\delta t$ of the first equation in the system $\tilde{\mathcal{S}}_d$. On the one hand, we write this latter equation at index $n-3$ obtaining

$$i\frac{\nabla\phi^{n-1} - \nabla\phi^{n-2}}{\delta t} = -\Delta\frac{\nabla\phi^{n-1} + \nabla\phi^{n-2}}{2} + \nabla(-\Delta^{-1})\operatorname{div}\left(\boldsymbol{\Phi}^{n-\frac{3}{2}}\right).$$

On the other hand we subtract the equation above from the first equation in the system $\tilde{\mathcal{S}}_d$ and get, after multiplication by $(2\delta t)^{-1}$,

$$\begin{aligned}
&i\,\frac{\frac{\nabla\phi^{n+1}-\nabla\phi^n}{\delta t} - \frac{\nabla\phi^{n-1}-\nabla\phi^{n-2}}{\delta t}}{2\delta t} + \Delta\left(\frac{\frac{\nabla\phi^{n+1}-\nabla\phi^n}{\delta t} + 2\frac{\nabla\phi^{n}-\nabla\phi^{n-1}}{\delta t} + \frac{\nabla\phi^{n-1}-\nabla\phi^{n-2}}{\delta t}}{4}\right)\\
&= \nabla(-\Delta^{-1})\operatorname{div}\left(\frac{\xi^{n+\frac{1}{2}} - \xi^{n-\frac{3}{2}}}{2\delta t}\,\frac{\nabla\phi^{n+1} + \nabla\phi^n + \nabla\phi^{n-1} + \nabla\phi^{n-2}}{4}\right) +\\
&+ \nabla(-\Delta^{-1})\operatorname{div}\left(\frac{\xi^{n+\frac{1}{2}} + \xi^{n-\frac{3}{2}}}{2}\,\frac{\frac{\nabla\phi^{n+1}-\nabla\phi^n}{\delta t} + 2\frac{\nabla\phi^{n}-\nabla\phi^{n-1}}{\delta t} + \frac{\nabla\phi^{n-1}-\nabla\phi^{n-2}}{\delta t}}{4}\right)\\
&= \nabla(-\Delta^{-1})\operatorname{div}\left(\Re\left(\boldsymbol{\psi}^{n-\frac{1}{2}}(\nabla\bar{\phi}^n + \nabla\bar{\phi}^{n-1})\right)\,\frac{\nabla\phi^{n+1} + \nabla\phi^n + \nabla\phi^{n-1} + \nabla\phi^{n-2}}{4}\right)\\
&+ \nabla(-\Delta^{-1})\operatorname{div}\left(\frac{\xi^{n+\frac{1}{2}} + \xi^{n-\frac{3}{2}}}{2}\,\frac{\frac{\nabla\phi^{n+1}-\nabla\phi^n}{\delta t} + 2\frac{\nabla\phi^{n}-\nabla\phi^{n-1}}{\delta t} + \frac{\nabla\phi^{n-1}-\nabla\phi^{n-2}}{\delta t}}{4}\right).
\end{aligned}$$

Eventually, setting $v^{n+\frac{1}{2}} = \boldsymbol{\psi}^{n+\frac{1}{2}} - \frac{\nabla\phi^{n+1}-\nabla\phi^n}{\delta t}$ and subtracting the last discrete equation from the second equation of the system $\tilde{\mathcal{S}}_d$ evaluated at index

$n-1$ we get

$$
\begin{aligned}
i\frac{v^{n+\frac{1}{2}}-v^{n-\frac{3}{2}}}{2\delta t} &= -\Delta\left(\frac{v^{n+\frac{1}{2}}+2v^{n-\frac{1}{2}}+v^{n-\frac{3}{2}}}{4}\right)\\
&+ \nabla\left(-\Delta^{-1}\right)\mathrm{div}\left(\frac{\xi^{n+\frac{1}{2}}+\xi^{n-\frac{1}{2}}}{2}\,\frac{v^{n+\frac{1}{2}}+2v^{n-\frac{1}{2}}+v^{n-\frac{3}{2}}}{4}\right).
\end{aligned}
$$

With initial data $v^{\frac{1}{2}}=v^{-\frac{1}{2}}=0$, this PDE has a trivial solution $v=0$. By uniqueness of solutions to this equation we obtain $\boldsymbol{\psi}^{n+\frac{1}{2}}=\frac{\nabla\phi^{n+1}-\nabla\phi^{n}}{\delta t}$ which is the first equality we want to show. We get the second equality observing that now we have $\frac{\xi^{k+\frac{1}{2}}-\xi^{k-\frac{3}{2}}}{2\delta t}=\frac{|\nabla\phi^{k}|^2-|\nabla\phi^{k-1}|^2}{\delta t}$. Summing up with respect to k leads to the desired equality and implies the equivalence of $\mathcal{S}_d$ and $\tilde{\mathcal{S}}_d$.

Now, we turn to the proof of existence and uniqueness of a solution of the system $\tilde{\mathcal{S}}_d$. It is based on the following discrete Duhamel formula for a solution of $\tilde{\mathcal{S}}_d$, which we obtain following the argumentation in [4].

$$
\tilde{\mathcal{S}}_d' : \begin{cases}
\nabla\phi^{n+2} = B^{n+2}\nabla\phi_0 - i\,\delta t\displaystyle\sum_{k=0}^{n+1} AB^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\mathrm{div}\left(\Phi^{k+\frac{1}{2}}\right),\\
\xi^{n+\frac{3}{2}} = \begin{cases} |\nabla\phi^0|^2 + 2\delta t\sum_{k=0}^{r} \Xi^{2k-\frac{1}{2}} & \text{if} \quad n=2r+1\ ,\\ |\nabla\phi^0|^2 + 2\delta t\sum_{k=0}^{r} \Xi^{2k+\frac{1}{2}} & \text{if} \quad n=2r\ ,\end{cases}\\
\boldsymbol{\psi}^{n+\frac{3}{2}} = \left(\mathcal{X}^{n+2}\boldsymbol{\psi}^{\frac{1}{2}} + \mathcal{X}^{n+1}B\boldsymbol{\psi}^{-\frac{1}{2}}\right)\\
\qquad\qquad - 2i\delta t\displaystyle\sum_{k=0}^{n} A\mathcal{X}^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\mathrm{div}\left(\Psi^{k+\frac{1}{2}}\right)\ .
\end{cases}
$$

We will use a fixed point argument to prove the existence of a unique solution to $\tilde{\mathcal{S}}_d'$, and therefore to $\tilde{\mathcal{S}}_d$. To this end we introduce the following notation,

$$
\begin{aligned}
(\nabla\phi)^N &= (\nabla\phi^2,\ldots,\nabla\phi^{N+1})\ , &\qquad (\nabla\tilde{\phi})^N &= (\nabla\tilde{\phi}^2,\ldots,\nabla\tilde{\phi}^{N+1})\ ,\\
(\xi)^N &= (\xi^{\frac{3}{2}},\ldots,\xi^{N+\frac{1}{2}})\ , & (\tilde{\xi})^N &= (\tilde{\xi}^{\frac{3}{2}},\ldots,\tilde{\xi}^{N+\frac{1}{2}})\ ,\\
(\boldsymbol{\psi})^N &= (\boldsymbol{\psi}^{\frac{3}{2}},\ldots,\boldsymbol{\psi}^{N+\frac{1}{2}})\ , & (\tilde{\boldsymbol{\psi}})^N &= (\tilde{\boldsymbol{\psi}}^{\frac{3}{2}},\ldots,\tilde{\boldsymbol{\psi}}^{N+\frac{1}{2}})\ .
\end{aligned}
$$

We shall prove that the mapping Λ defined as

$$
\begin{aligned}
\Lambda:\quad & \mathfrak{H}_N\times\mathfrak{H}_N\times\mathfrak{H}_N & \longrightarrow\quad & \mathfrak{H}_N\times\mathfrak{H}_N\times\mathfrak{H}_N\\
& \left((\nabla\tilde{\phi})^N,(\tilde{\xi})^N,(\tilde{\boldsymbol{\psi}})^N\right) & \longmapsto\quad & \left((\nabla\phi)^N,(\xi)^N,(\boldsymbol{\psi})^N\right)
\end{aligned}
$$

has a unique fixed point in the space $\mathfrak{H}_N^3 := \ell^\infty(0,N;H^m)^3$. We obtain the fixed point iteration Λ adapting the Duhamel formula $\tilde{\mathcal{S}}_d'$ as

$$\Lambda: \begin{cases} \nabla\phi^{n+2} = B^{n+2}\nabla\phi_0 - i\,\delta t\displaystyle\sum_{k=0}^{n+1} AB^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\mathrm{div}\left[\tilde{\xi}^{k+\frac12}\,\frac{\nabla\tilde{\phi}^{k+1}+\nabla\tilde{\phi}^{k}}{2}\right], \\ \xi^{n+\frac32} = \begin{cases} |\nabla\phi^0|^2 + 4\delta t\sum_{k=0}^r \Re\left[\tilde{\boldsymbol{\psi}}^{2k-\frac12}\,\frac{\nabla\tilde{\phi}^{2k}+\nabla\tilde{\phi}^{2k-1}}{2}\right] & \text{if} \quad n=2r+1\,, \\ |\nabla\phi^0|^2 + 4\delta t\sum_{k=0}^r \Re\left[\tilde{\boldsymbol{\psi}}^{2k+\frac12}\,\frac{\nabla\tilde{\phi}^{2k+1}+\nabla\tilde{\phi}^{2}k}{2}\right] & \text{if} \quad n=2r\,, \end{cases} \\ \boldsymbol{\psi}^{n+\frac32} = \left(\mathcal{X}^{n+2}\boldsymbol{\psi}^{\frac12} + \mathcal{X}^{n+1}B\boldsymbol{\psi}^{-\frac12}\right) \\ \quad - 2i\delta t\displaystyle\sum_{k=0}^{n} A\mathcal{X}^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\mathrm{div}\left[\frac{\tilde{\xi}^{k+\frac32}+\tilde{\xi}^{k-\frac12}}{2}\,\frac{\tilde{\boldsymbol{\psi}}^{k+\frac32}+2\tilde{\boldsymbol{\psi}}^{k+\frac12}+\tilde{\boldsymbol{\psi}}^{k-\frac12}}{4}\right] \\ \quad - 4i\delta t\displaystyle\sum_{k=0}^{n} A\mathcal{X}^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\mathrm{div}\left[\Re\left(\tilde{\boldsymbol{\psi}}^{k+\frac12}\,\frac{\nabla\tilde{\phi}^{k+1}+\nabla\tilde{\phi}^{k}}{2}\right)\times\right. \\ \qquad\qquad\qquad\left.\times\,\frac{\nabla\tilde{\phi}^{k+2}+\nabla\tilde{\phi}^{k+1}+\nabla\tilde{\phi}^{k}+\nabla\tilde{\phi}^{k-1}}{4}\right]. \end{cases}$$

The set of initial data we use is the one of $\tilde{\mathcal{S}}_d$,

$$\tilde{\xi}^{-\frac12} = \xi^{-\frac12},\quad \tilde{\xi}^{\frac12} = \xi^{\frac12},\quad \tilde{\boldsymbol{\psi}}^{-\frac12} = \boldsymbol{\psi}^{-\frac12},$$
$$\tilde{\boldsymbol{\psi}}^{\frac12} = \boldsymbol{\psi}^{\frac12},\quad \nabla\tilde{\phi}^0 = \nabla\phi^0,\quad \nabla\tilde{\phi}^1 = \nabla\phi^1.$$

Now, let us pick $R = 2\left[\|\nabla\phi^0\|_{H^m} + \|\nabla\phi^0\|_{H^m}^2 + \|\boldsymbol{\psi}^{-\frac12}\|_{H^m}\right]$ and assume that $(\nabla\tilde{\phi})^N, (\tilde{\boldsymbol{\psi}})^N$ and $(\tilde{\xi})^N$ are in the closed ball of radius R in $\mathfrak{H}_N$. Then, using (3.3), the Lemmas 2 and 3 and the fact that $H^m(\mathbb{R}^3)$ is an algebra as soon as $m > \frac32$, we obtain that there are constants $c_1, c_2, c_3 > 0$ independent of n and δt such that

$$\begin{aligned} &\|\nabla\phi^{n+2}\|_{H^m} \le \|\nabla\phi_0\|_{H^m} + \,c_1\,T_{\delta t}\,\|(\tilde{\xi})^N\|_{\mathfrak{H}_N}\,\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}\,, \\ &\|\xi^{n+\frac32}\|_{H^m} \le \|\nabla\phi_0\|_{H^m}^2 + \,c_3\,T_{\delta t}\,\|(\tilde{\boldsymbol{\psi}})^N\|_{\mathfrak{H}_N}\,\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}\,, \\ &\|\boldsymbol{\psi}^{n+\frac32}\|_{H^m} \le \|\boldsymbol{\psi}^{-\frac12}\|_{H^m} + \,c_2\,T_{\delta t}\,\|(\tilde{\boldsymbol{\psi}})^N\|_{\mathfrak{H}_N}\left(\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}^2 + \|(\tilde{\xi})^N\|_{\mathfrak{H}_N}\right). \end{aligned} \tag{3.4}$$

We conclude that there exists a function $\kappa = \kappa(R)$, which is monotone in R such that

$$\|(\nabla\phi)^N\|_{\mathfrak{H}_N} + \|(\boldsymbol{\psi})^N\|_{\mathfrak{H}_N} + \|(\xi)^N\|_{\mathfrak{H}_N} \le \frac{R}{2} + \kappa(R)\,T_{\delta t}\,,$$

so that if we pick $T_{\delta t}$ small enough, then Λ maps the ball of radius R in $(\mathfrak{H}_N)^3$ into itself.

The same argument with extra algebraic manipulation (triangular inequality) shows that there exists a possibly even smaller $T_{\delta t}$ such that Λ is a strict contraction which implies the existence and uniqueness of a solution $((\nabla\phi)^N, (\boldsymbol{\psi})^N, (\xi)^N)$ to $\tilde{\mathcal{S}}_d$ subject to the initial data listed above.

At this level, we know that $(\nabla\phi)^N \in \ell^\infty(0, N; H^m)$. Since all the functions we used to construct the solution $(\nabla\phi)^N$ are elements of $\mathcal{V}$ (cf. [5]) it holds that $(\nabla\phi)^N \in \ell^\infty(0, N; \mathcal{V})$. Therefore, all elements of the sequence $(\nabla\phi)^N$ are gradients of functions in $\mathcal{D}'$. The sequence of those functions is denoted by $(\phi)^N$. Thus the Gagliardo–Nirenberg–Sobolev inequality implies that $(\phi)^N \in L^6(\mathbb{R}^3)$. As the initial datum ξ_0 is continuous, the continuity of the elements of $(\phi)^N$ follows, eventually we see that $(\phi)^N$ is in fact in $\ell^\infty(0, N, \mathcal{H}^m)$. Thus the proof of Theorem 2 is complete.

4 Convergence

Theorem 2 provides us with the local-in-time well-posedness of the discrete system $\mathcal{S}_d$ associated to the continuous system $\mathcal{S}'_c$. The last point to make clear in order to finish the proof of the Theorem 3 is the convergence of the discrete unique solution to the unique continuous solution. The proof is achieved in a standard way, that is by comparing the discrete Duhamel formula to the continuous one. Let us first start with the Duhamel formula associated to the continuous system $\tilde{\mathcal{S}}_c$,

$$\begin{cases} \nabla\phi(t,x) = U(t)\nabla\phi_0 - i\displaystyle\int_0^t U(t-s)\nabla(-\Delta^{-1})\,\mathrm{div}\,(\Phi(s,x))\,ds\,, \\ \xi(t,x) = |\nabla\phi_0|^2 + \displaystyle\int_0^t \Xi(s,x)\,ds\,, \\ \boldsymbol{\psi}(t,x) = U(t)\boldsymbol{\psi}(t=0) - i\displaystyle\int_0^t U(t-s)\nabla\,(-\Delta^{-1})\,\mathrm{div}\,(\Psi(s,x))\,ds\,. \end{cases} \tag{4.1}$$

Comparing this formulation with $\tilde{\mathcal{S}}'_d$ we see that it is rather straightforward to prove the convergence of $\nabla\phi^{n+2}$ to $\nabla\phi$ and $\xi^{n+\frac{3}{2}}$ to ξ.

Let us now turn to the proof of the convergence of $\boldsymbol{\psi}^{n+\frac{3}{2}}$ to $\boldsymbol{\psi}$. First of all, we observe that due to (3.3) the contribution of the initial data part to the convergence is not problematic. Unfortunately, the operator $A\mathcal{X}^{n+1-k}$ in $\tilde{\mathcal{S}}'_d$ is not consistent with the free propagator $U(t)$. Indeed, the bounded operator $A\mathcal{X}^{n+1-k}$ (cf. Lemma 3) generates two different semigroups depending on the parity of the exponent $n+1-k$. In order to get more insight one uses that

$\mathcal{X}^k = \sum_{l=1}^{k} (-1)^{l-1} B^{k-l}$ and obtains after some calculation

$$\sum_{k=0}^{n} A\mathcal{X}^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Psi^{k+\frac{1}{2}}\right) =$$
$$= \begin{cases} \sum_{l=0}^{r} 2\delta t A B^{2l+1}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Psi^{\frac{1}{2}} + \sum_{q=0}^{r-l-1} \delta t \frac{\Psi^{2q+\frac{5}{2}} - \Psi^{2q+\frac{3}{2}}}{\delta t}\right) + \\ \quad + \sum_{l=0}^{r} 2\delta t A B^{2l}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\sum_{q=0}^{r-l} \delta t \frac{\Psi^{2q+\frac{3}{2}} - \Psi^{2q+\frac{1}{2}}}{\delta t}\right) \qquad n = 2r+1\ , \\ \sum_{l=0}^{r-1} 2\delta t A B^{2l+1}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\sum_{q=0}^{r-l-1} \delta t \frac{\Psi^{2q+\frac{3}{2}} - \Psi^{2q+\frac{1}{2}}}{\delta t}\right) + \\ \quad + \sum_{l=0}^{r} 2\delta t A B^{2l}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Psi^{\frac{1}{2}} + \sum_{q=0}^{r-l-1} \delta t \frac{\Psi^{2q+\frac{5}{2}} - \Psi^{2q+\frac{3}{2}}}{\delta t}\right) \qquad n = 2r\ , \end{cases}$$

which allows to define $\hat{\Psi}^{k+\frac{1}{2}}$ such that

$$\boldsymbol{\psi}^{n+\frac{3}{2}} = B^{n+2}\boldsymbol{\psi}^{-\frac{1}{2}} - i\delta t \sum_{k=0}^{n} A B^{n+1-k}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\hat{\Psi}^{k+\frac{1}{2}}\right)\ . \tag{4.2}$$

This suggests that the continuous Duhamel formula in (4.1) for $\boldsymbol{\psi}(t,x)$ should be interpreted as

$$\boldsymbol{\psi}(t,x) = U(t)\boldsymbol{\psi}(t=0) - i\int_0^t U(t-s)\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\int_0^s \partial_t \Psi(\tilde{s},x)\,d\tilde{s}\right) ds\ .$$

Therefore we see immediately that now the time derivatives of $\boldsymbol{\theta}(t,x) := \partial_t\boldsymbol{\psi}(t,x)$ and $\zeta(t,x) := \partial_t \xi(t,x)$ are involved. We extend the continuous system $\tilde{\mathcal{S}}_c$ by these extra quantities and their associated evolution equations,

$$\tilde{\mathcal{S}}_c^{\mathrm{ext}}:\quad \begin{cases} \partial_t \zeta = \mathcal{Z}\ , \\ i\partial_t\boldsymbol{\theta} = -\Delta\boldsymbol{\theta} + \nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Theta\right)\ , \end{cases}$$

where

$$\begin{aligned} \mathcal{Z} &:= 2\left(\Re\left(\left(\boldsymbol{\theta}\nabla\bar{\phi}\right)\right) + |\boldsymbol{\psi}|^2\right)\ , \\ \Theta &:= 2\left(\Re(\boldsymbol{\theta}\nabla\bar{\phi})\nabla\phi + |\boldsymbol{\psi}|^2\nabla\phi + \Re(\boldsymbol{\psi}\nabla\bar{\phi})\boldsymbol{\psi} + \zeta\boldsymbol{\psi} + \xi\,\boldsymbol{\theta}\right)\ . \end{aligned}$$

On the discrete level, let $\boldsymbol{\theta}^{n+1} := \frac{\boldsymbol{\psi}^{n+\frac{3}{2}} - \boldsymbol{\psi}^{n+\frac{1}{2}}}{\delta t}$ and $\zeta^{n+1} := \frac{\xi^{n+\frac{3}{2}} - \xi^{n+\frac{1}{2}}}{\delta t}$ and after some calculations we obtain the following discrete version of the above continuous system

$$\tilde{\mathcal{S}}_d^{\mathrm{ext}}:\ \begin{cases} \dfrac{\zeta^{n+1} - \zeta^{n-1}}{2\delta t} = \mathcal{Z}^n\ , \\ i\dfrac{\boldsymbol{\theta}^{n+1} - \boldsymbol{\theta}^{n-1}}{2\delta t} = -\Delta\dfrac{\boldsymbol{\theta}^{n+1} + \boldsymbol{\theta}^{n-1}}{2} + \nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\Theta^n\right)\ , \end{cases}$$

where

$$
\begin{aligned}
\Theta^n = 2\Bigg[& \left(\Re\left(\boldsymbol{\theta}^n \frac{\nabla\bar{\phi}^{n+1} + 2\nabla\bar{\phi}^n + \nabla\bar{\phi}^{n-1}}{4} \right) + \left| \frac{\boldsymbol{\psi}^{n+\frac{1}{2}} + \boldsymbol{\psi}^{n-\frac{1}{2}}}{2} \right|^2 \right) \times \\
& \times \frac{\nabla\phi^{n+2} + 2\nabla\phi^{n+1} + 2\nabla\phi^n + 2\nabla\phi^{n-1} + \nabla\phi^{n-2}}{8} \Bigg] \\
& + 2\left[\Re\left(\frac{\boldsymbol{\psi}^{n+\frac{1}{2}} \frac{\nabla\bar{\phi}^{n+1} + \nabla\bar{\phi}^n}{2} + \boldsymbol{\psi}^{n-\frac{1}{2}} \frac{\nabla\bar{\phi}^n + \nabla\bar{\phi}^{n-1}}{2}}{2} \right) \times \right. \\
& \left. \times \frac{\boldsymbol{\psi}^{n+\frac{3}{2}} + \boldsymbol{\psi}^{n+\frac{1}{2}} + \boldsymbol{\psi}^{n-\frac{1}{2}} + \boldsymbol{\psi}^{n-\frac{3}{2}}}{4} \right] \qquad (4.3) \\
& + \frac{\zeta^{n+1} + \zeta^{n-1}}{2} \frac{\boldsymbol{\psi}^{n+\frac{3}{2}} + 3\boldsymbol{\psi}^{n+\frac{1}{2}} + 3\boldsymbol{\psi}^{n-\frac{1}{2}} + \boldsymbol{\psi}^{n-\frac{3}{2}}}{8} \\
& + \frac{\xi^{n+\frac{3}{2}} + \xi^{n+\frac{1}{2}} + \xi^{n-\frac{1}{2}} + \xi^{n-\frac{3}{2}}}{4} \frac{\boldsymbol{\theta}^{n+1} + 2\boldsymbol{\theta}^n + \boldsymbol{\theta}^{n-1}}{4}, \\
\mathcal{Z}^n = 2\Re & \left(\boldsymbol{\theta}^n \frac{\nabla\bar{\phi}^{n+1} + 2\nabla\bar{\phi}^n + \nabla\bar{\phi}^{n-1}}{4} \right) + \left| \frac{\boldsymbol{\psi}^{n+\frac{1}{2}} + \boldsymbol{\psi}^{n-\frac{1}{2}}}{2} \right|^2 .
\end{aligned}
$$

First of all, we have to prove the well-posedness of this discrete system. We introduce $\tilde{A} = (1 - i\delta t\Delta)^{-1}$ and $\tilde{B} = \tilde{A}(1 + i\delta t\Delta)$. These operators obviously enjoy an equivalent version of Lemma 3. As usual, we start by writing the discrete Duhamel Formula.

$$
\tilde{\mathcal{S}}_d'^{\text{ext}} : \begin{cases} \zeta^n = \begin{cases} \zeta^{-1} + 2\delta t \sum_{k=0}^{r} \mathcal{Z}^{2k} & \text{if} \quad n = 2r+1 , \\ \zeta^0 + 2\delta t \sum_{k=0}^{r} \mathcal{Z}^{2k-1} & \text{if} \quad n = 2r , \end{cases} \\ \boldsymbol{\theta}^n = \begin{cases} \tilde{B}^r \boldsymbol{\theta}^1 - 2i\delta t \sum_{k=0}^{r-1} \tilde{A}\tilde{B}^{r-k-1} \nabla(-\Delta^{-1}) \operatorname{div}\left(\Theta^{2k+2}\right) & \text{if} \quad n = 2r+1 , \\ \tilde{B}^r \boldsymbol{\theta}^0 - 2i\delta t \sum_{k=0}^{r-1} \tilde{A}\tilde{B}^{r-k-1} \nabla(-\Delta^{-1}) \operatorname{div}\left(\Theta^{2k+1}\right) & \text{if} \quad n = 2r . \end{cases} \end{cases}
$$

The proof of local-in-time existence and uniqueness of solutions to this discrete Duhamel system $\{\tilde{\mathcal{S}}_d', \tilde{\mathcal{S}}_d'^{\text{ext}}\}$ is analogous to the one of the system $\tilde{\mathcal{S}}_d'$. For that purpose, we introduce the following notation

$$
\begin{aligned}
(\zeta)^N &= (\zeta^1, \ldots, \zeta^{N+1}) , & (\tilde{\zeta})^N &= (\tilde{\zeta}^1, \ldots, \tilde{\zeta}^{N+1}) , \\
(\boldsymbol{\theta})^N &= (\boldsymbol{\theta}^1, \ldots, \boldsymbol{\theta}^{N+1}) , & (\tilde{\boldsymbol{\theta}})^N &= (\tilde{\boldsymbol{\theta}}^1, \ldots, \tilde{\boldsymbol{\theta}}^{N+1}) ,
\end{aligned}
$$

and extend the mapping Λ,

$$
\begin{aligned}
\Lambda^{\text{ext}} : \quad & \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N & \longrightarrow \quad & \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N \times \mathfrak{H}_N \\
& \left((\nabla\tilde{\phi})^N, (\tilde{\xi})^N, (\tilde{\boldsymbol{\psi}})^N, (\tilde{\zeta})^N, (\tilde{\boldsymbol{\theta}})^N\right) & \longmapsto \quad & \left((\nabla\phi)^N, (\xi)^N, (\boldsymbol{\psi})^N, (\zeta)^N, (\boldsymbol{\theta})^N\right)
\end{aligned}
$$

The space is given by $\mathfrak{H}_N := \ell^\infty(0, N; H^m)$ and the mapping Λ^{ext} is explicitly defined as follows

$$\Lambda^{\text{ext}}\begin{cases}\left((\nabla\phi)^N,(\xi)^N,(\boldsymbol{\psi})^N\right)=\Lambda\left((\nabla\tilde{\phi})^N,(\tilde{\xi})^N,(\tilde{\boldsymbol{\psi}})^N\right)\\ \zeta^n=\begin{cases}\zeta^{-1}+2\delta t\sum_{k=0}^{r}\tilde{\mathcal{Z}}^{2k} & \text{if} \quad n=2r+1\,,\\ \zeta^0+2\delta t\sum_{k=0}^{r}\tilde{\mathcal{Z}}^{2k-1} & \text{if} \quad n=2r\,.\end{cases}\\ \boldsymbol{\theta}^n=\begin{cases}\tilde{B}^r\boldsymbol{\theta}^1-2i\delta t\sum_{k=0}^{r-1}\tilde{A}\tilde{B}^{r-k-1}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\tilde{\Theta}^{2k+2}\right) & \text{if} \quad n=2r+1\,,\\ \tilde{B}^r\boldsymbol{\theta}^0-2i\delta t\sum_{k=0}^{r-1}\tilde{A}\tilde{B}^{r-k-1}\,\nabla\left(-\Delta^{-1}\right)\operatorname{div}\left(\tilde{\Theta}^{2k+1}\right) & \text{if} \quad n=2r\,.\end{cases}\end{cases}$$

The nonlinear terms $\tilde{\Theta}$ and $\tilde{\mathcal{Z}}$ are given by (4.3) evaluated at $(\nabla\tilde{\phi})^N$, $(\tilde{\boldsymbol{\psi}})^N$, $(\tilde{\xi})^N$, $(\tilde{\zeta})^N$ and $(\tilde{\boldsymbol{\theta}})^N$. Next, let us pick

$$R_2:=2\Big[\|\nabla\phi_0\|_{H^m}+\|\nabla\phi_0\|_{H^m}^2+\|\boldsymbol{\psi}^{-\frac{1}{2}}\|_{H^m}+ \\ +\max(\|\boldsymbol{\theta}^0\|_{H^m},\|\boldsymbol{\theta}^1\|_{H^m})+\max(\|\zeta^0\|_{H^m},\|\zeta^{-1}\|_{H^m})\Big].$$

We recall that H^m is an algebra if $m>\frac{3}{2}$. Therefore, for all $m>\frac{3}{2}+4$ (in order to ensure the regularity of $\boldsymbol{\psi}$ and $\boldsymbol{\theta}$) there are constants $c_4,c_5>0$ such that

$$\|\boldsymbol{\theta}^n\|_{H^m}\le\max(\|\boldsymbol{\theta}^0\|_{H^m},\|\boldsymbol{\theta}^1\|_{H^m})+c_4\,T_{\delta t}\Bigg(\|(\tilde{\boldsymbol{\theta}})^N\|_{\mathfrak{H}_N}\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}^2+ \\ +\|(\tilde{\boldsymbol{\psi}})^N\|_{\mathfrak{H}_N}^2\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}+\|(\tilde{\zeta})^N\|_{\mathfrak{H}_N}\|(\tilde{\boldsymbol{\psi}})^N\|_{\mathfrak{H}_N}+\|(\tilde{\xi})^N\|_{\mathfrak{H}_N}\|(\tilde{\boldsymbol{\theta}})^N\|_{\mathfrak{H}_N}\Bigg).$$

$$\|\zeta^n\|_{H^m}\le\max(\|\zeta^0\|_{H^m},\|\zeta^{-1}\|_{H^m})+c_5\,T_{\delta t}\left(\|(\tilde{\boldsymbol{\theta}})^N\|_{\mathfrak{H}_N}\|(\nabla\tilde{\phi})^N\|_{\mathfrak{H}_N}+\|(\tilde{\boldsymbol{\psi}})^N\|_{\mathfrak{H}_N}^2\right).$$

Therefore, using also the inequalities (3.4) there is a function $\kappa_2=\kappa_2(R_2)$, which is monotone in R_2 such that

$$\|(\nabla\phi)^N\|_{\mathfrak{H}_N}+\|(\boldsymbol{\psi})^N\|_{\mathfrak{H}_N}+\|(\boldsymbol{\theta})^N\|_{\mathfrak{H}_N}+\|(\xi)^N\|_{\mathfrak{H}_N}+\|(\zeta)^N\|_{\mathfrak{H}_N}\le\frac{R_2}{2}+\kappa_2(R_2)\,T_{\delta t}$$

so that if we pick $T_{\delta t}$ small enough, then Λ^{ext} maps the ball of radius R_2 in $(\mathfrak{H}_N)^5$ into itself. Again, it is easy to show that there exists a $T_{\delta t}$ (even smaller if necessary) such that Λ^{ext} is a strict contraction which leads to the existence and uniqueness of the solution $((\nabla\phi)^N,(\xi)^N,(\boldsymbol{\psi})^N,(\zeta)^N,(\boldsymbol{\theta})^N)\in\mathfrak{H}_N^5$ to the system above.

Next, we finish the proof of convergence and we shall focus on the case of n even for simplicity, our estimates apply exactly for the other case and the argument goes *mutatis mutandis*. To this end and in order to be able to pass the the limit we need a C^2 regularity for the continuous solution $\nabla\phi$. Following Corollary 1, we let then $m>\frac{3}{2}+4$ so that $\nabla\phi\in C^2([0,T(\phi_0)[,\mathcal{H}^m)$. Next, for all $t\in[t_n,t_{n+1}]$, let

$$\begin{aligned}
\nabla\phi_{\delta t}(t,x)&=\nabla\phi^n(x) & \Phi_{\delta t}(t,x)&=\Phi^{n+\frac{1}{2}}(x)\\
\xi_{\delta t}(t,x)&=\xi^{n+\frac{1}{2}}(x) & \Xi_{\delta t}(t,x)&=\Xi^{n+\frac{1}{2}}(x)\\
\boldsymbol{\psi}_{\delta t}(t,x)&=\boldsymbol{\psi}^{n+\frac{1}{2}}(x) & \hat{\Psi}_{\delta t}(t,x)&=\hat{\Psi}^{n+\frac{1}{2}}(x)\\
\zeta_{\delta t}(t,x)&=\zeta^n(x) & \mathcal{Z}_{\delta t}(t,x)&=\Phi^n(x)\\
\boldsymbol{\theta}_{\delta t}(t,x)&=\boldsymbol{\theta}^n(x) & \Theta_{\delta t}(t,x)&=\Theta^n(x)
\end{aligned}$$

and introduce the following short notations for the continuous and approximating versions of the initial datum, the solution and the right hand side in the respective Duhamel formula

$$\begin{aligned}
Q_0 &:= (\nabla\phi_0, |\nabla\phi_0|^2, \partial_t\nabla\phi(t=0), \partial_t\xi(t=0), \partial_t^2\nabla\phi(t=0)),\\
Q_{\delta t,0} &:= (\nabla\phi_0, |\nabla\phi_0|^2, \boldsymbol{\psi}^{-\frac{1}{2}}, \zeta^0, \boldsymbol{\theta}^0),\\
Q &:= (\nabla\phi, \xi, \partial_t\nabla\phi, \partial_t\xi, \partial_t^2\nabla\phi),\\
Q_{\delta t} &:= (\nabla\phi_{\delta t}, \xi_{\delta t}, \boldsymbol{\psi}_{\delta t}, \zeta_{\delta t}, \boldsymbol{\theta}_{\delta t}),\\
\mathcal{F} &:= (\,\nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\varPhi, -i\varXi, \nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\varPsi, -i\mathcal{Z}, \nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\varTheta),\\
\mathcal{F}_{\delta t} &:= (\,\nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\varPhi_{\delta_t}, -i\varXi_{\delta_t}, \nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\hat{\varPsi}_{\delta_t}, -i\mathcal{Z}_{\delta_t}, \nabla\,(-\varDelta^{-1})\,\mathrm{div}\,\varTheta_{\delta_t})\;.
\end{aligned}$$

We also aggregate the propagators for the various continuous and discrete quantities using the symbols

$$\mathcal{G} = (A, I, A, I, \tilde{A})\;, \quad \mathcal{U} = (e^{it\varDelta}, I, e^{it\varDelta}, I, e^{it\varDelta})\;, \quad \mathcal{U}_{\delta t} = (AB^n, 1, AB^r, 1, \tilde{A}\tilde{W}^n)\;,$$

where $n = 2r$ and $t_n \le t < t_{n+1}$. The solutions Q and $Q_{\delta t}$ are then characterized by the following Duhamel formula

$$\begin{aligned}
Q &= \mathcal{U}(t)Q_0 - i\int_0^t \mathcal{U}(t-s)\mathcal{F}(s)\,ds\;,\\
Q_{\delta t} &= \mathcal{U}_{\delta t}(t)Q_{\delta t,0} - i\int_0^t \mathcal{G}\mathcal{U}_{\delta t}(t-s)\,\mathcal{F}_{\delta t}(s)\,ds\;.
\end{aligned}$$

We intend to estimate the difference $Q(t) - Q_{\delta t}(t)$ in $L^\infty([0, N\delta t], (H^m)^5)$. First of all, we have clearly the following

$$\begin{aligned}
&\|Q - Q_{\delta t}\|_{L^\infty([0,N\delta t],H^m)} \le \|\mathcal{U}Q_0 - \mathcal{U}_{\delta t}Q_{\delta t,0}\|_{L^\infty([0,N\delta t];(H^m)^5)}\\
&\quad + \left\|\int_0^t \left[\mathcal{U}(t-\tau)\mathcal{F}(Q)(\tau) - \mathcal{G}\mathcal{U}_{\delta t}(t-\tau)\mathcal{F}_{\delta_t}(\tau)\right]\,d\tau\right\|_{L^\infty([0,N\delta t];(H^m)^5)}\;.
\end{aligned} \tag{4.4}$$

Indeed, with the triangular inequality, one writes

$$\begin{aligned}
&\|\mathcal{U}Q_0 - \mathcal{U}_{\delta t}Q_{\delta t,0}\|_{L^\infty([0,N\delta t];(H^m)^5)} \le\\
&\qquad \le \|[\mathcal{U} - \mathcal{U}_{\delta t}]\,Q_0\|_{L^\infty([0,N\delta t];(H^m)^5)} +\\
&\qquad + \|\mathcal{U}_{\delta t}\,[Q_0 - Q_{\delta t,0}]\|_{L^\infty([0,N\delta t];(H^m)^5)} \to 0 \quad \text{as} \quad \delta t \to 0\;,
\end{aligned}$$

where the convergence of the first difference in norm is due to convergence of operators according to Lemma 3. The convergence of the second expression is a consequence of the definition of the scheme $\tilde{\mathcal{S}}_d$ which implies that $\nabla\phi^1 \to \nabla\phi^0$ as $\delta t \to 0$ and therefore

$$\begin{aligned}
\boldsymbol{\psi}^{\frac{1}{2}} &= \frac{\nabla\phi^1 - \nabla\phi^0}{\delta t} = -\varDelta\frac{\nabla\phi^1 + \nabla\phi^0}{2} + \nabla\,(-\varDelta^{-1})\,\mathrm{div}\left(\varPhi^{\frac{1}{2}}\right) \to\\
&\qquad \to -\varDelta\nabla\phi|_{t=0} + \nabla\,(-\varDelta^{-1})\,\mathrm{div}\,(\varPhi)|_{t=0} = -i\partial_t\nabla\phi|_{t=0}
\end{aligned}$$

as $\delta t \to 0$, where we used $\nabla\phi \in C^2((0,T), H^m(\mathbb{R}^3))$. This proves the convergence of the first term in the right-hand side of (4.4). The second term is treated as follows. For simplicity we fix $t = t_{n+1}$ and estimate

$$\begin{aligned}
&\left\| \int_0^{t_{n+1}} \left[\mathcal{U}(t_{n+1}-\tau)\mathcal{F}(\tau) - \mathcal{G}\mathcal{U}_{\delta t}(t_{n+1}-\tau)Q_{\delta t}(\mathcal{F}_{\delta_t})(\tau)\right] d\tau \right\|_{(H^m)^5} \\
&\quad\leq \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \left[\mathcal{G}\mathcal{U}_{\delta t}(t_{n+1}-t_l)\mathcal{F}_{\delta t}(t_l) - \mathcal{U}(t_{n+1}-\tau)\mathcal{F}(\tau)\right] d\tau \right\|_{(H^m)^5} \\
&\quad\leq \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \left[\mathcal{G}\mathcal{U}_{\delta t}(t_{n+1}-t_l) - \mathcal{U}(t_{n+1}-t_l)\right] \mathcal{F}_{\delta t}(t_l) d\tau \right\|_{(H^m)^5} \\
&\quad+ \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \mathcal{U}(t_{n+1}-t_l)\left[\mathcal{F}_{\delta t}(t_l) - \mathcal{F}(\tau)\right] d\tau \right\|_{(H^m)^5} \\
&\quad+ \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \left[\mathcal{U}(t_{n+1}-t_l) - \mathcal{U}(t_{n+1}-\tau)\right] \mathcal{F}(\tau) d\tau \right\|_{(H^m)^5} .
\end{aligned}$$

Observe that t_l is completely independent of τ and depends only on l and δt. Again since $\mathcal{G} \longrightarrow 1$ and $\mathcal{U}_{\delta t} \xrightarrow[\delta t \to 0]{} \mathcal{U}$ for the strong topology of operators in $(H^m)^5$, we have

$$\sup_{0\leq n\leq N} \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \left[\mathcal{G}\mathcal{U}_{\delta t}(t_{n+1}-t_l) - \mathcal{U}(t_{n+1}-t_l)\right] \mathcal{F}_{\delta t}(t_l) d\tau \right\|_{(H^m)^5} \xrightarrow[\delta t\to 0]{} 0 ,$$

$$\sup_{0\leq n\leq N} \sum_{l=0}^{n} \left\| \int_{t_l}^{t_{l+1}} \left[\mathcal{U}(t_{n+1}-t_l) - \mathcal{U}(t_{n+1}-\tau)\right] \mathcal{F}(\tau) d\tau \right\|_{(H^m)^5} \xrightarrow[\delta t\to 0]{} 0 .$$

For the remaining term following [6, 4] we introduce $\overline{\mathcal{F}}_{\delta t}(t_l)$ by evaluating the residual terms (3.1) and (4.3) at $Q(t_l)$ instead of $Q_{\delta t}(t_l)$. Hence it holds

$$\begin{aligned}
&\left\| \int_{t_l}^{t_{l+1}} \mathcal{U}(t_{n+1}-t_l)\left[\mathcal{F}_{\delta t}(\tilde{\tau}) - \mathcal{F}(\tau)\right] d\tau \right\|_{(H^m)^5} \leq \\
&\qquad \leq \delta t \left(\left\|\mathcal{F}_{\delta t}(\tilde{\tau}) - \overline{\mathcal{F}}_{\delta t}(\tilde{\tau})\right\|_{(H^m)^5} + \sup_{\tau\in[t_l,t_{l+1}]} \|\overline{\mathcal{F}}_{\delta t}(t_l) - \mathcal{F}(\tau)\|_{(H^m)^5} \right).
\end{aligned}$$

Now, on the one hand, since $\nabla\phi \in C^2([0, T(\phi_0)[, H^m)$, we have

$$\delta t \sum_{l=0}^{N} \sup_{\tau\in[t_l,t_{l+1}]} \|\overline{\mathcal{F}}_{\delta t}(t_l) - \mathcal{F}(\tau)\|_{(H^m)^5} \xrightarrow[\delta t\to 0]{} 0.$$

On the other hand using the uniform estimates on Q and $Q_{\delta t}$ in $[0, N\delta t]$ we conclude that there is a constant such that

$$\left\|\mathcal{F}_{\delta t}(t_l) - \overline{\mathcal{F}}_{\delta t}(t_l)\right\|_{(H^m)^5} \leq \text{Const.} \, \|Q_{\delta t} - Q\|_{L^\infty([0,N\delta t];(H^m)^5)} .$$

Eventually combining these results with (4.4) we obtain

$$\|Q - Q_{\delta t}\|_{L^\infty([0,N\delta t];(H^m)^5)} \leq o(1) + \text{Const.}\, N\,\delta t \|Q - Q_{\delta t}\|_{L^\infty([0,N\delta t];(H^m)^5)}.$$

Thus, if we pick N such that Const. $N\,\delta t < 1$, then we get

$$\|Q - Q_{\delta t}\|_{L^\infty([0,N\delta t];(H^m)^5)} \xrightarrow[\delta t \to 0]{} 0.$$

Now, iterating the argument on the whole interval $[0, T]$ by considering now initial data at $N\delta t$, we get the lower semicontinuity of the existence time $T_{\delta t}$ as $\delta t \longrightarrow 0$ and the convergence on $[0, \tau]$ for all $0 \leq \tau \leq T$. The proof of Theorem 3 is finished.

5 Conclusion

In this paper we have analyzed a relaxation-type scheme for a nonlinear Schrödinger equation. We have demonstrated that the proposed scheme conserves *mass* and *energy* as opposed to classical schemes like splitting, Runge-Kutta, symplectic, etc. that fail in preserving these important physical observables. Furthermore, we have proved the well posedness of the semi-discretized system and that its solution converges towards the solution of the continuous problem in suitable Sobolev spaces. Let us also mention that the scheme avoids a costly numerical treatment of the nonlinearity and doesn't require a particular space discretization. The scheme is inspired by [4] where the case of the cubic NLS is treated, it can be easily adapted to the Davey-Stewartson system.

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