Chapter 1

Modulated solitons algorithms for nonlinear Schrödinger equations

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We discuss in this paper new algorithms for the nonlinear cubic Schrödinger equation, based on the representation by modulated solitons in interactions. We consider the general idea of modulation and calculate explicitly the evolution of a single soliton for which the evolution system of the modulation parameters form a completely integrable system. We then discuss the numerical approximation of nonlinear interactions of several modulated solitons through the Dirac-Frenkel variational principle. Numerical examples illustrate that the method yields very satisfying results in the case of weak interactions, and allows the computations of interacting solitons in the whole space without a full grid of discretization.

1. Introduction

We consider in this work the cubic nonlinear Schrödinger equation with harmonic potential:

$$\left| \begin{array}{l} i\partial_t u(t,x) = -\Delta u(t,x) + |x|^2 u(t,x) + \mu |u(t,x)|^2 u(t,x), \\ u(0,\cdot) = U_0, \end{array} \right. \tag{1}$$

where $(t,x) \in \mathbb{R}_+ \times \mathbb{R}^d$, $\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}$, $|x|^2 = x_1^2 + \cdots + x_d^2$ and $\mu \in \mathbb{R}$, and U_0 a smooth given function. In the case $\mu < 0$ the equation is said to be *focusing*, and if $\mu > 0$ it is *defocusing*. When $\mu = 0$ it is the well-known harmonic oscillator. The cubic nonlinearity is treated for its physical importance, but the method presented should be adaptable to any type of nonlinearity. Equation (1) is also sometimes called the "Gross-Pitaevskii" equation.

The relevance of the Schrödinger equation in a multi-dimensional context arises from its physical nature. For instance, if one considers the

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variable space of two coherent particles moving in three-dimensional space, we get $d = 6$ (see [1]). We also refer to [2] for a good introduction to the high-dimensional linear Schrödinger equation in molecular dynamics (i.e. in the case $\mu = 0$ but with potentials with complex structures). The cubic nonlinearity is usually used when studying the Bose-Einstein condensates in the two- or three-dimensional context. The nonlinear Schrödinger equation can also be recovered from the Maxwell equation in specific settings, for instance in the field propagation of a single-mode optical fiber [3, 4]. We refer to [5, 6] for extensive studies of the nonlinear Schrödinger equation with general local nonlinearities.

There has been also many works dedicated to the numerical approximation of (1). Grid-based methods are very efficient at recovering the effects of the nonlinearity because they do not assume any information about the solution, but they are also very difficult to use in practice since the numerical grids need to be very fine, see e.g. [7–10]. Moreover, a space discretization has to be combined with a time discretization and time splitting method are usually employed, see [11, 12, 16]. In molecular dynamics, grid-free base methods have been extensively studied by considering approximation of (1) by modulated Gaussian. This is very efficient and widely applied in the case of the linear Schrödinger equation with potential, in particular in problems coming from molecular dyanmics (see e.g. [2, 13–15, 17, 18]).

In the nonlinear situation, the computation of *interacting solitons* has known many interesting progresses in physics and in numerical analysis [9, 35]. Similarly, from the theoretical point of view very recent works [19, 20] suggest to consider solutions ψ of (1) that are sum of N modulated functions, which write as:

$$\psi(t,x) \approx u(t,x) := \sum_{j=1}^{N} u^j(t,x), \tag{2}$$

where

$$u^j(t,x) := \frac{1}{L^j} e^{i\gamma^j + iL^j\beta^j\cdot y^j - i\frac{B^j}{4}|y^j|^2} v^j(t,y^j), \quad \text{with} \quad y^j := \frac{x - X^j}{L^j}, \tag{3}$$

and $N \in \mathbb{N}^*$. Such a representation means that we seek the solution of the equation on a manifold made of modulated functions v^j. The time dependence of the parameters $A^j, L^j, B^j, X^j, \beta^j, \gamma^j$ has not been written in (3) for the sake of clarity, but it is one of the main ingredients of the approach. More precisely, the core idea is to plug the ansatz (2) into (1) in order to obtain ODEs for the parameters by projection onto the manifold.

The choice of the function v^j is fundamental. In the linear case, *i.e.* when the cubic nonlinearity is replaced by some multiplication with a potential, and particularly in the semi-classical regime, the v^j are chosen as Gaussian functions. Such techniques have been called *Variational Gaussian wave packets* and have been extensively analyzed, see for instance [2], with many refinements and application in the field of Chemical Physics [13, 14, 21–23].

In the nonlinear setting, we can also choose the v^j Gaussian as in the linear case, and consider the approximation by the Dirac-Frankel principle, but a more natural choice consists in taking v^j as solitons *i.e.* functions Q solution of the following eigenproblem:

$$-\Delta Q(x) + |x|^2 Q(x) + \mu |Q(x)|^2 Q(x) = \omega Q(x), \quad x \in \mathbb{R}^d, \tag{4}$$

for which some symmetry can be imposed (typically radially symmetric). Note that ω is essentially piloted by the L^2 norm of Q, that can be chosen arbitrarily. We refer to [33, 34] for the existence theory of such solution. In particular we can find radial solution that are positive (ground states) by variational or ordinary differential equation techniques. We can also construct for $|\mu| \ll 1$ solutions to (4) that are close to Gaussian or Hermite functions when $\mu \to 0$ by bifurcation and the Lyapunov-Schmidt method. Considering a manifold of the form (2) made of modulated solitons $v^j := Q^j$ for some j is thus a natural generalization to the nonlinear case of the classical Gaussian algorithms used in the linear case and in molecular dynamics.

Let us now explain the main ideas underlying the full modulation (3) – developed in various works, see for instance [19, 20] and the references therein – and why it is particularly adapted to the nonlinear case.

Consider for instance the case of one function v, *i.e.* $N = 1$. When plugging the ansatz (3) into (1), we obtain an equation of the form

$$L^2 i\partial_t v + \Delta_y v - |y|^2 v - \mu |v|^2 v + R(t; y, \partial_y) v = 0, \tag{5}$$

where $R(t; y, \partial_y)$ is a quadratic operator in y and ∂_y, which depends on time t through the parameters $P = (\gamma, X, \beta, B, L)$ and their time derivatives with respect to t. See (10) for more precise detail. It is then possible to choose the parameters in such a way that for instance $R(t; y, \partial_y)v = \omega v$ for some $\omega \in \mathbb{R}$, and to take $v = Q$ a soliton solution of the stationary equation (4) which will be a constant in time solution of (5). This yields a differential system to be solved by the parameters $P = (\gamma, X, \beta, B, L)$ which is given below by (16). It turns out that these equations form a *completely integrable Poisson system* that can be solved explicitly.

This kind of approach has been used successfully in various situations from a theoretical point of view, see [19, 20, 24, 25] and the references therein. Typically, when $N \geq 2$, several modulated solitons interact and this can produce finite time blow-up, periodic or quasi-periodic in time solutions, or growth of Sobolev norm phenomena. A large part of the analysis relies on the ability of calculating nonlinear interactions between two modulated solitons that are possibility weakly interacting. Note that the calculation of soliton interaction can be done explicitly for instance in an integrable situation, e.g. the Szegö equation [26]. But in the general case, we have to rely on numerical simulations.

Another by-product of these modulation techniques in 2D is to make a link between (1) on a finite time interval and the Schrödinger equation without harmonic potential

$$i\partial_s\psi + \Delta_x\psi = \mu\psi|\psi|^2, \quad x \in \mathbb{R}^d \tag{6}$$

on an unbounded time interval. In this case, the modulation equations generate the so-called *lens* transform, see for instance [6]. Note that our algorithms could also be applied to the latter equation but we will restrict our analysis to the Harmonic case. Let us note as well that such modulation techniques can also be related with the families of exact splitting introduced in [12].

In this work, we retain the idea of approximating solutions to (1) by modulating the parameters L^j, B^j, X^j, β^j, γ^j in combination with the Dirac-Frenkel principle consisting in projecting the equation on the manifold (3).

As we have explained above, for $N = 1$ the equation will be exact up to the numerical discretization of the equation (4). In the general case $N \geq 2$, the only difficulty comes from the calculation of the interactions terms: if $u = f + g$, the nonlinearity $|u|^2u$ can be split into two terms. The first one is $|f|^2f + |g|^2g$, and by the soliton definition it can be taken into account "explicitely". The second term is the interaction term of the form $f^2\bar{g}$ or $|g|^2f$, or any combination of three solitons in the case $N \geq 3$. To be evaluated, these term have to be projected on the modulated soliton manifold. We approximate the interaction terms by using the Dirac-Frenkel principle using grid discretization that will behave favorably for weak interactions (when the solitons are distant for instance).

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2. General modulation

2.1. *Notations*

We set

$$(f,g)_{L^2} = \int f\overline{g}, \quad \|f\|^2_{L^2} = (f,f)_{L^2}, \quad \langle f,g\rangle = \mathrm{Re}\int f\overline{g}, \tag{7}$$

the latter bracket being the real scalar product on complex functions of $L^2(\mathbb{R}^d)$ viewed as a real Hilbert space. We can find for instance in [5] or [6] that the following (real) quantities are preserved along solutions of (1):

- L^2 norm: $\|\psi\|^2_{L^2}$,
- Energy: $\mathcal{E}(t) = \frac{1}{2}\left(-\Delta\psi + |x|^2\psi, \psi\right)_{L^2} + \frac{\mu}{4}\left(|\psi|^2\psi,\psi\right)_{L^2}$
- Momentum: $m(t) = \left(\mathcal{E}(t) - \|x\psi\|^2_{L^2}\right)^2 + \left(\Im\left[\int x\cdot\nabla\psi\overline{\psi}\right]\right)^2$.

Let $X, \beta \in \mathbb{R}^d$, $\gamma, B \in \mathbb{R}$ and $L > 0$. We set

$$P = (\gamma, X, \beta, B, L) \in \mathbb{R}^{2d+2} \times \mathbb{R}_+, \tag{8}$$

the set of modulation parameters, and we define an operator $\mathcal{M}_P : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$, where for $f \in L^2(\mathbb{R}^d)$,

$$(\mathcal{M}_P f)(t,x) := \frac{1}{L}\exp\left\{i\gamma + iL\beta\cdot y + \frac{iB}{2}|y|^2\right\} f(t,y), \quad y := \frac{x-X}{L}. \tag{9}$$

When several different modulations will be involved, we will denote them by exponents: for instance, $\mathcal{M}_{P^j}$ will be the j-th modulation operator, associated to a set of modulation parameters P^j (see (8)). The modulation parameters follow the same rule, and to denote a squared modulation parameter, we will write for example $(L^j)^2$. For a vector, its k-th component will be denoted by the index $_k$. For example X^j_k denotes the k-th component of the modulation parameter X^j. We also write

$$M_P(x) := \frac{1}{L}\exp\left\{i\gamma + iL\beta\cdot\frac{x-X}{L} + \frac{iB}{2}\left|\frac{x-X}{L}\right|^2\right\}.$$

Let us remark that we have

$$\|(\mathcal{M}_P f)(x)\|^2_{L^2} = \frac{1}{L^2}\int_{\mathbb{R}^d}|f|^2(\frac{x}{L})dx = L^{d-2}\|f\|^2_{L^2}$$

Hence for a given f we can fix the L^2 norm of $(\mathcal{M}_P f)(x)$ by scaling L, except in dimension 2 where this norm have to be fixed by f itself.

2.2. *Single modulation*

We now search u solution of the nonlinear Schrödinger equation as a modulated function v, i.e.

$$u(t,x) = (\mathcal{M}_{P(t)}v)(t,x) = M_{P(t)}(x)v(t,y(t,x)), \quad y(t,x) = \frac{x-X}{L}.$$

We will reformulate the nonlinear Schrödinger equation with unknown $u(t,x)$ as another nonlinear equation with unknown $v(t,y(t,x))$. In this new nonlinear equation the modulation parameters will appear, as well as their time derivative. By correctly choosing the time evolution of these parameters, it will be shown that the function v can simply be expressed.

Proposition 1. *Let* $P(t)$ *be a set of time dependent parameters* (8) *and* $u(t,x) = (\mathcal{M}_{P(t)}v)(t,x)$. *We have*

$$\begin{aligned}&(i\partial_t u + \Delta_x u - |x|^2 u - \mu|u|^2 u)(t,x) = M_{P(t)}(x)\\ &\times \left[\begin{array}{c} i\partial_t + i\left(-\dfrac{\dot{L}}{L} + \dfrac{B}{L^2}d\right) - \dot{\gamma} + \beta\cdot\dot{X} - |X|^2 - |\beta|^2 \\ + \left(-L\dot{\beta} + \dfrac{B}{L}\dot{X} - 2\dfrac{B}{L}\beta - 2LX\right)\cdot y \\ + \left(\dfrac{B\dot{L}}{L} - \dfrac{\dot{B}}{2} - \dfrac{B^2}{L^2} - L^2\right)|y|^2 + i\left(2\dfrac{\beta}{L} - \dfrac{\dot{X}}{L}\right)\cdot\nabla \\ +i\left(2\dfrac{B}{L^2} - \dfrac{\dot{L}}{L}\right) y\cdot\nabla + \dfrac{1}{L^2}\Delta_y - \dfrac{\mu}{L^2}|v(t,y(t,x))|^2 \end{array}\right] v(t,y(t,x)). \quad (10)\end{aligned}$$

Proof. We start by computing, in dimension $d \geq 1$,

$$\Delta_x u = \frac{e^{i\gamma}}{L^2}\Delta_y\left[e^{iL\beta\cdot y + i\frac{B}{2}|y|^2}v(t,y)\right].$$

After differentiating with respect to the k-th coordinate, we get for $k = 1,\dots,d$,

$$\partial_{y_k}\left[e^{iL\beta\cdot y+i\frac{B}{2}|y|^2}v\right] = e^{iL\beta\cdot y+i\frac{B}{2}|y|^2}\left[\partial_{y_k}v + i\left(L\beta_k + By_k\right)v\right]. \quad (11)$$

Differentiating again with respect to the k-th coordinate:

$$\begin{aligned}&\partial^2_{y_k}\left[e^{iL\beta\cdot y+i\frac{B}{2}|y|^2}v\right]\\ &\quad = e^{iL\beta\cdot y+i\frac{B}{2}|y|^2}\left[\begin{array}{c}\partial^2_{y_k}v + i\left(L\beta_k + By_k\right)\partial_{y_k}v + iBv \\ +i\left(L\beta_k+By_k\right)\left[\partial_{y_k}v + i\left(L\beta_k+By_k\right)v\right]\end{array}\right]\\ &\quad = e^{iL\beta\cdot y+i\frac{B}{2}|y|^2}\left[\begin{array}{c}\partial^2_{y_k}v + 2i\left(L\beta_k+By_k\right)\partial_{y_k}v \\ +iBv - \left(L\beta_k+By_k\right)^2 v\end{array}\right]. \quad (12)\end{aligned}$$

By summing (12) over $k = 1, \dots, d$, we get

$$\begin{aligned}&\Delta_x u = M_{P(t)}(x)\\ &\times \left[\frac{1}{L^2}\Delta_y v + 2i\left(\frac{\beta}{L} + \frac{B}{L^2}y\right)\cdot\nabla v + i\frac{Bd}{L^2}v - \left|\beta + \frac{B}{L}y\right|^2\right]\\ &= M_{P(t)}(x)\\ &\times \left[\frac{1}{L^2}\Delta_y v + 2i\left(\frac{\beta}{L} + \frac{B}{L^2}y\right)\cdot\nabla v + i\frac{Bd}{L^2}v\right.\\ &\quad\left. - \left(|\beta|^2 + 2\frac{B}{L}\beta\cdot y + \frac{B^2}{L^2}|y|^2\right)v\right].\end{aligned}$$

We have

$$\begin{aligned}-|x|^2 u &= -M_{P(t)}(x)\,|Ly + X|^2\,v\\ &= M_{P(t)}(x)\left(-L^2|y|^2 - 2LX\cdot y - |X|^2\right)v,\end{aligned}$$

thus

$$(\Delta_x - |x|^2)u = M_{P(t)}(x) \times \begin{bmatrix} \frac{1}{L^2}\Delta_y v + 2i\left(\frac{\beta}{L} + \frac{B}{L^2}y\right)\cdot\nabla v + i\frac{Bd}{L^2}v \\ + \left(-|\beta|^2 - 2\frac{B}{L}\beta\cdot y - \frac{B^2}{L^2}|y|^2 - L^2|y|^2 - 2LX\cdot y - |X|^2\right)v \end{bmatrix}, \tag{13}$$

We now differentiate u with respect to time t:

$$\begin{aligned}&\partial_t u(t,x) = \partial_t\left(e^{i\gamma + iL\beta\cdot y(t,x) + i\frac{B}{2}|y(t,x)|^2}\frac{1}{L}v(t, y(t,x))\right)\\ &= e^{i\gamma + iL\beta\cdot y + i\frac{B}{2}|y|^2}\left[-\frac{\dot{L}}{L^2}v(t,y) + \frac{1}{L}\left(\partial_t v + \frac{dy}{dt}\cdot\nabla v\right)\right]\\ &+ iM_{P(t)}(x)\left[\dot{\gamma} + L\dot{\beta}\cdot y + \dot{L}\beta\cdot y + L\beta\cdot\frac{dy}{dt} + \frac{\dot{B}}{2}|y|^2 + B\frac{dy}{dt}\cdot y\right]v(t,y).\end{aligned}$$

with the notation $y = y(t,x)$ for which we have

$$\frac{dy}{dt} = -\frac{\dot{X}}{L} - \frac{\dot{L}}{L}y.$$

Thus

$$\begin{aligned}&\partial_t u(t,x) = M_{P(t)}(x)\left[-\frac{\dot{L}}{L} + \partial_t - \frac{\dot{X}}{L}\cdot\nabla - \frac{\dot{L}}{L}y\cdot\nabla\right]v\\ &+ iM_{P(t)}(x)\left[\dot{\gamma} + \left(L\dot{\beta} - \frac{B\dot{X}}{L}\right)\cdot y - \beta\cdot\dot{X} + \left(\frac{\dot{B}}{2} - \frac{B\dot{L}}{L}\right)|y|^2\right]v(t,y).\end{aligned}$$

Hence,

$$i\partial_t u = M_{P(t)}(x) \begin{bmatrix} i\partial_t - i\dfrac{\dot{L}}{L} - \dot{\gamma} + \beta \cdot \dot{X} \\ + \left(-L\dot{\beta} + \dfrac{B}{L}\dot{X}\right) \cdot y \\ + \left(\dfrac{B\dot{L}}{L} - \dfrac{\dot{B}}{2}\right) |y|^2 \\ -i\dfrac{\dot{X}}{L} \cdot \nabla - i\dfrac{\dot{L}}{L} y \cdot \nabla \end{bmatrix} v(t, y). \tag{14}$$

Finally, the nonlinearity satisfies

$$|u|^2 u = M_{P(t)}(x) \frac{1}{L^2} |v|^2 v.$$

Gathering the previous calculation yields (10). ☐

Once we have this equation, we are free to choose the parameters as we wish. Until now, the parameters have been completely free, with no condition whatsoever on them or their time derivatives. The main idea is to now choose conditions so that (10) becomes an equation on v in variables (t, y) that is "easy" to solve.

2.3. *Two-dimensional solitons*

From now on we assume $d = 2$. Let Q a soliton associated to an eigenvalue ω, i.e. any solution to (4):

$$-\Delta_z Q(z) + |z|^2 Q(z) + \mu |Q(z)|^2 Q(z) = \omega Q(z),$$

and define $v(t, y) := Q(y)$. Note that for $\mu = 0$, the equation (1) is the linear Harmonic oscillator, and the previous PDEs is solved by Hermite functions. We can also construct solutions for $|\mu| \ll 1$ close to any Hermite function by perturbation, see [34]. We have immediatly that

$$i\partial_t v = 0$$

and

$$\frac{1}{L^2} \Delta_y v(y) - \frac{|y|^2}{L^2} v(y) - \frac{\mu}{L^2} |v(y)|^2 v(y) = -\frac{\omega}{L^2} v(y).$$

Therefore, with such v, we get

$$
\begin{aligned}
&(i\partial_t u + \Delta_x u - |x|^2 u - \mu |u|^2 u)(t,x) = M_{P(t)}(x)\\
&\times \left[\begin{array}{c}
i\left(-\frac{\dot L}{L}+\frac{B}{L^2}d\right) - \dot\gamma + \beta\cdot\dot X - |X|^2 - |\beta|^2 - \frac{\omega}{L^2}\\
+\left(-L\dot\beta + \frac{B}{L}\dot X - 2\frac{B}{L}\beta - 2LX\right)\cdot y \\
+\left(\frac{B\dot L}{L} - \frac{\dot B}{2} - \frac{B^2}{L^2} - L^2 + \frac{1}{L^2}\right)|y|^2 \\
+i\left(2\frac{\beta}{L}-\frac{\dot X}{L}\right)\cdot\nabla + i\left(2\frac{B}{L^2}-\frac{\dot L}{L}\right) y\cdot\nabla
\end{array}\right] v(t,y(t,x)).
\end{aligned}
\tag{15}
$$

We then chose the time derivatives of the modulation parameters as follows:

$$
\left|\begin{array}{l}
\frac{\dot L}{L} - 2\frac{B}{L^2} = 0\\
-\dot\gamma + \beta\cdot\dot X - |X|^2 - |\beta|^2 - \frac{\omega}{L^2} = 0\\
-L\dot\beta + \frac{B}{L}\dot X - 2\frac{B}{L}\beta - 2LX = 0\\
\frac{B\dot L}{L} - \frac{\dot B}{2} - \frac{B^2}{L^2} - L^2 + \frac{1}{L^2} = 0\\
2\frac{\beta}{L} - \frac{\dot X}{L} = 0,
\end{array}\right.
\iff
\left|\begin{array}{l}
\dot L = 2\frac{B}{L}\\
\dot\gamma = |\beta|^2 - |X|^2 - \frac{\omega}{L^2}\\
\dot\beta = -2X\\
\dot B = 2\frac{B^2+1}{L^2} - 2L^2\\
\dot X = 2\beta.
\end{array}\right.
\tag{16}
$$

Finally, we obtain a solution of the equation (1) of the form

$$
u(t,x) = \frac{1}{L} e^{i\gamma + iL\beta\cdot y + i\frac{B}{2}|y|^2} Q(y).
$$

where $y = \frac{x - X(t)}{L(t)}$ and the parameters $P(t)$ evolve according to the previous set of ordinary differential equations.

2.4. *Modulation equations*

In this section we want to find explicit expressions for the modulation parameters solving (16). Note that the couples (X,β) and (L,B) can be written as Hamiltonian systems:

$$
\left|\begin{array}{l}
\dot X = \partial_\beta \mathcal{R}(X,\beta)\\
\dot\beta = -\partial_X \mathcal{R}(X,\beta)
\end{array}\right.
\quad \text{and} \quad
\left|\begin{array}{l}
\dot L = L\partial_B \mathcal{E}(L,B)\\
\dot B = -L\partial_L \mathcal{E}(L,B),
\end{array}\right.
$$

where

$$\mathcal{R}(X,\beta) = |X|^2 + |\beta|^2 \quad \text{and} \quad \mathcal{E}(L,B) = \frac{B^2+1}{L^2} + L^2.$$

The couple (L,B) is a non-canonical Hamiltonian system, so we write $k = \log L$ and obtain

$$\left|\begin{aligned} &\dot{k} = \partial_B \mathcal{E}(k,B) \\ &\dot{B} = -\partial_k \mathcal{E}(k,B), \end{aligned}\right.$$

with $\mathcal{E}(k,B) = (B^2+1)e^{-2k} + e^{2k}$. Finally, the canonical Hamiltonian system is

$$\left|\begin{aligned} &\dot{X} = \partial_\beta \mathcal{H} \\ &\dot{\beta} = -\partial_X \mathcal{H} \\ &\dot{k} = \partial_B \mathcal{H} \\ &\dot{B} = -\partial_k \mathcal{H}, \end{aligned}\right.$$

where the Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H}(X,\beta,k,B) = \mathcal{R}(X,\beta) + \mathcal{E}(k,B) = |X|^2 + |\beta|^2 + (B^2+1)e^{-2k} + e^{2k}.$$

Note that this system is a completely integrable system (see for instance [28, 32] and the reference therein) and we can calculate explicitly the corresponding action-angle variables:

Lemma 1 (Action-angle variables and exact update formulas). *There exists a symplectic change of variable* $(X,B,k,\beta) \mapsto (h,a,\xi,\theta) \in \mathbb{R} \times \mathbb{R}^d \times [0,2\pi] \times [0,2\pi]^d$*, such that the Hamiltonian in these variables is given by*

$$E(h,a,\xi,\theta) = 4h + 2a, \tag{17}$$

so that the flow in variable (h,a,ξ,θ) *is given by*

$$\left|\begin{aligned} &a(t) = a(0), \\ &\theta(t) = \theta(0) + 2t, \end{aligned}\right. \quad \textit{and} \quad \left|\begin{aligned} &h(t) = h(0), \\ &\xi(t) = \xi(0) + 4t. \end{aligned}\right. \tag{18}$$

Moreover, solutions to the dynamical system (16) *are given by the explicit* *formulas:*

$$\begin{aligned}
e^{2k(t)} &= L(t)^2 = 2h(t) - \cos(\xi(t))\sqrt{4h(t)^2 - 1},\\
B(t) &= \sin(\xi(t))\sqrt{4h(t)^2 - 1},\\
X_i(t) &= \sin(\theta_i(t))\sqrt{2a_i(t)}, \quad i = 1, \dots, d,\\
\beta_i(t) &= \cos(\theta_i(t))\sqrt{2a_i(t)}, \quad i = 1, \dots, d,\\
\gamma(t) &= \sum_{l=1}^{d} \frac{a_l}{2}\left[\sin(2\theta_l(t)) - \sin(2\theta_l(0))\right]\\
&\quad + \frac{\omega}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(t)}{2}\right)\right)\\
&\quad - \frac{\omega}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(0)}{2}\right)\right) + m_t\frac{\pi}{2},
\end{aligned} \tag{19}$$

where, if $m_0 \in \mathbb{Z}$ *is such that* $\frac{\xi(0)}{2} \in m_0\pi + \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$, *then* $m_t \in \mathbb{Z}$ *is defined by* $\frac{\xi(t)}{2} \in (m_0 - m_t)\pi + \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$.

Proof. For the (X, β) part, it suffices to check that the change of variable $(X, \beta) \mapsto (a, \theta)$ defined by

$$X_i = \sqrt{2a_i}\sin(\theta_i) \quad \text{and} \quad \beta_i = \sqrt{2a_i}\cos(\theta_i) \qquad i = 1, \dots, d,$$

is symplectic and that

$$X_i = \sqrt{2a_i(0)}\sin(2t + \theta_i(0)) \quad \text{and} \quad \beta_i = \sqrt{2a_i(0)}\cos(2t + \theta_i(0))$$

are solutions. Thus,

$$a_i(t) = a_i(0) \qquad \text{and} \qquad \theta_i(t) = \theta_i(0) + 2t. \tag{20}$$

For the (k, B) part we use the method of generating functions, described e.g. in [28, Sect. VI.5]. We can express B in terms of k and the Hamiltonian $\mathcal{E}$, so that on the set $\{B > 0\}$ we have:

$$B = \sqrt{e^{2k}\mathcal{E} - e^{4k} - 1}. \tag{21}$$

This equality holds for $e^{2k} \in [e^{2k_0}, e^{2k_1}]$, where e^{2k_0}, e^{2k_1} are the reals roots of the polynomial $-z^2 + \mathcal{E}z - 1$,

$$e^{2k_0} = \frac{1}{2}\left(\mathcal{E} - \sqrt{\mathcal{E}^2 - 4}\right), \quad e^{2k_1} = \frac{1}{2}\left(\mathcal{E} + \sqrt{\mathcal{E}^2 - 4}\right). \tag{22}$$

In order to obtain a symplectic change of variables, we look for a function $S(k, \mathcal{E})$ such that

$$B = -\frac{\partial S}{\partial k}(k, \mathcal{E}).$$

We easily obtain $S(k,\mathcal{E})$, by integrating on $[k_0,k]$:

$$S(k,\mathcal{E}) = -\int_{k_0}^{k} \sqrt{e^{2z}\mathcal{E} - e^{4z} - 1}\,dz.$$

The variable ϕ which makes the mapping $(B,k) \mapsto (\phi,\mathcal{E})$ symplectic is defined by

$$\phi = \frac{\partial S}{\partial \mathcal{E}}(k,\mathcal{E}) = -\frac{1}{2}\int_{k_0}^{k} \frac{e^{2z}}{\sqrt{e^{2z}\mathcal{E} - e^{4z} - 1}}dz.$$

We then have

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = -\frac{1}{2}\frac{e^{2k}\dot{k}}{\sqrt{e^{2k}\mathcal{E} - e^{4k} - 1}} = -\frac{1}{2}\frac{e^{2k}\partial_B \mathcal{E}}{B} = -\frac{1}{2}\frac{e^{-2k}2Be^{2k}}{B} = -1.$$

We now proceed to obtaining an explicit expression for ϕ:

$$\begin{aligned}
\phi &= -\frac{1}{2}\int_{k_0}^{k} \frac{e^{2z}}{\sqrt{e^{2z}\mathcal{E} - e^{4z} - 1}}dz = -\frac{1}{4}\int_{e^{2k_0}}^{e^{2k}} \frac{1}{\sqrt{\mathcal{E}u - u^2 - 1}}du \\
&= -\frac{1}{4\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\int_{e^{2k_0}}^{e^{2k}} \frac{1}{\sqrt{1 - \left(\frac{u - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right)^2}}du = -\frac{1}{4}\int_{\frac{e^{2k_0} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}}^{\frac{e^{2k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}} \frac{1}{\sqrt{1 - r^2}}dr.
\end{aligned}$$

Recall the definition (22) of k_0, which yields

$$e^{2k_0} - \frac{\mathcal{E}}{2} = -\sqrt{\frac{\mathcal{E}^2}{4} - 1}.$$

Therefore,

$$\begin{aligned}
\phi &= -\frac{1}{4}\int_{-1}^{\frac{e^{2k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}} \frac{1}{\sqrt{1 - r^2}}dr = -\frac{1}{4}\left(\arcsin\left(\frac{e^{2k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right) + \frac{\pi}{2}\right) \\
&= -\frac{1}{4}\arcsin\left(\frac{e^{2k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right) - \frac{\pi}{8} \in \left[-\frac{\pi}{4}, 0\right].
\end{aligned}$$

We want the angle variable to lie in $[-\pi,\pi]$ so the above expression describes an eighth of a period. But we are only considering the set $\{B > 0\}$, thus the angle ξ we are looking for must lie only in $[0,\pi]$. Hence we set $(\xi,h) = (-4\phi, \mathcal{E}/4)$ and let the Hamiltonian $\mathcal{E}(\xi,h) = 4h$ with a slight abuse of notation. It is then clear that $\frac{\mathrm{d}h}{\mathrm{d}t} = 0$ and $\frac{\mathrm{d}\xi}{\mathrm{d}t} = 4$. Moreover,

$$\xi = \arcsin\left(\frac{e^{2k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right) + \frac{\pi}{2} \in [0,\pi], \tag{23}$$

and hence

$$\frac{e^{2k}-\frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4}-1}}=\sin\left(\xi-\frac{\pi}{2}\right)=-\cos\left(\xi\right).$$

We obtain

$$\begin{aligned}e^{2k}=L^2=\frac{\mathcal{E}}{2}-\cos(\xi)\sqrt{\frac{\mathcal{E}^2}{4}-1}&=2h-\cos(\xi)\sqrt{4h^2-1}\\&=2h\left(1-\cos(\xi)\sqrt{1-\frac{1}{4h^2}}\right).\end{aligned}$$

With this formula, we have

$$0<L^2<4h=\mathcal{E},$$

and (21) becomes

$$\begin{aligned}B&=\sqrt{\mathcal{E}e^{2k}-e^{4k}-1}=\sqrt{4he^{2k}-(e^{2k})^2-1}=\sqrt{(4h^2-1)\sin^2(\xi)}\\&=\sin(\xi)\sqrt{4h^2-1},\end{aligned}$$

where the last equality holds for $\xi\in[0,\pi]$.

We can now integrate the equation on γ, using direct integration:

$$\begin{aligned}&\int_0^t\left[|\beta(\tau)|^2-|X(\tau)|^2\right]d\tau=\int_0^t\left\{\sum_{l=1}^d 2a_l\cos(\theta_l(\tau))^2-\sum_{l=1}^d 2a_l\sin(\theta_l(\tau))^2\right\}d\tau\\&=\int_0^t 2\sum_{l=1}^d a_l\left(\cos(\theta_l(\tau))^2-\sin(\theta_l(\tau))^2\right)d\tau=\int_0^t\sum_{l=1}^d 2a_l\cos(2\theta_l(\tau))d\tau\\&=\sum_{l=1}^d\frac{a_l}{2}\left[\sin(2\theta_l(t))-\sin(2\theta_l(0))\right],\end{aligned}$$

where the last equality has been obtained using (20). We compute

$$\begin{aligned}\int_0^t\frac{1}{L(\tau)^2}dt&=\int_0^t\frac{1}{\underbrace{2h(0)}_{=:c_1}-\underbrace{\sqrt{4h(0)^2-1}}_{=:c_2}\cos(\xi(0)+4r)}dr\\&=\int_0^t\frac{1}{c_1-c_2\cos(\xi(0)+4r)}dr=\frac{1}{4}\int_{\xi(0)}^{\xi(0)+4t}\frac{1}{c_1-c_2\cos(\tau)}d\tau.\end{aligned}$$

Recall the following trigonometric identity:

$$\cos(2\tau)=\frac{1-\tan(\tau)^2}{1+\tan(\tau)^2},\quad \tau\in\mathbb{R},$$

hence

$$\begin{aligned}
&\int_0^t \frac{1}{c_1 - c_2\cos(\xi(0) - 4\tau)}d\tau \\
&= \frac{1}{4}\int_{\xi(0)}^{\xi(0)+4t} \frac{1}{c_1 - c_2\frac{1-\tan(\tau/2)^2}{1+\tan(\tau/2)^2}}d\tau \\
&= \frac{1}{4}\int_{\xi(0)}^{\xi(0)+4t} \frac{1+\tan(\tau/2)^2}{c_1(1+\tan(\tau/2)^2) - c_2(1-\tan(\tau/2)^2)}d\tau \\
&= \frac{1}{4}\int_{\xi(0)}^{\xi(0)+4t} \frac{1+\tan(\tau/2)^2}{(c_1+c_2)\tan(\tau/2)^2 + c_1 - c_2}d\tau \\
&= \frac{1}{4(c_1-c_2)}\int_{\xi(0)}^{\xi(0)+4t} \frac{1+\tan(\tau/2)^2}{\frac{c_1+c_2}{c_1-c_2}\tan(\tau/2)^2 + 1}d\tau \\
&= \frac{1}{2(c_1-c_2)}\int_{\frac{\xi(0)}{2}}^{\frac{\xi(0)}{2}+2t} \frac{1+\tan(\tau)^2}{\frac{c_1+c_2}{c_1-c_2}\tan(\tau)^2 + 1}d\tau \\
&= \frac{1}{2(c_1-c_2)}\int_{\frac{\xi(0)}{2}}^{\frac{\xi(0)}{2}+2t} \frac{\frac{d}{d\tau}(\tan(\tau))}{\frac{c_1+c_2}{c_1-c_2}\tan(\tau)^2 + 1}d\tau \\
&= \frac{1}{2(c_1-c_2)}\frac{1}{\sqrt{\frac{c_1+c_2}{c_1-c_2}}}\int_{\frac{\xi(0)}{2}}^{\frac{\xi(0)}{2}+2t} \frac{\frac{d}{d\tau}\left(\sqrt{\frac{c_1+c_2}{c_1-c_2}}\tan(\tau)\right)}{\left[\sqrt{\frac{c_1+c_2}{c_1-c_2}}\tan(\tau)\right]^2 + 1}d\tau.
\end{aligned}$$

Moreover, $(c_1-c_2)(c_1+c_2) = c_1^2 - c_2^2 = (2h)^2 - (4h^2-1) = 1$ and $c_1 - c_2 > 0$, thus $\sqrt{\frac{c_1+c_2}{c_1-c_2}} = (c_1+c_2)$ and

$$\int_0^t \frac{1}{L(\tau)^2}d\tau = \frac{1}{2}\int_{\frac{\xi(0)}{2}}^{\frac{\xi(0)}{2}+2t} \frac{\frac{d}{d\tau}\left((c_1+c_2)\tan(\tau)\right)}{\left((c_1+c_2)\tan(\tau)\right)^2 + 1}d\tau.$$

Now let $m_0 \in \mathbb{Z}$ such that $\frac{\xi(0)}{2} \in m_0\pi + \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$, and $m_t \in \mathbb{Z}$ such that $\frac{\xi(t)}{2} \in (m_0 - m_t)\pi + \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$. We recall that $\xi(t) = \xi(0) + 4t$. Then

$$\begin{aligned}
&\int_0^t \frac{1}{L(\tau)^2}d\tau = \frac{1}{2}\int_{\frac{\xi(0)}{2}}^{\frac{\xi(0)}{2}+2t} \underbrace{\frac{\frac{d}{d\tau}\left((c_1+c_2)\tan(\tau)\right)}{\left((c_1+c_2)\tan(\tau)\right)^2 + 1}}_{=:f(\tau)}d\tau \\
&= \frac{1}{2}\int_{\frac{\xi(0)}{2}}^{m_0\pi+\frac{\pi}{2}} f(\tau)d\tau + \frac{1}{2}\int_{(m_0+1)\pi-\frac{\pi}{2}}^{(m_0+1)\pi+\frac{\pi}{2}} f(\tau)d\tau + \cdots + \frac{1}{2}\int_{(m_0+m_t)\pi-\frac{\pi}{2}}^{\frac{\xi(0)}{2}+2t} f(\tau)d\tau.
\end{aligned}$$

For $m \in \mathbb{Z}$, we have

$$\begin{aligned}\int_{m\pi-\frac{\pi}{2}}^{m\pi+\frac{\pi}{2}} f(\tau)d\tau &= \left[\arctan\left((c_1+c_2)\tan(\tau)\right)\right]_{m\pi-\frac{\pi}{2}}^{m\pi+\frac{\pi}{2}} \\ &= \left[\arctan\left((c_1+c_2)\tan(\tau)\right)\right]_{-\frac{\pi}{2}}^{\frac{\pi}{2}} = \pi.\end{aligned}$$

Now write $\widetilde{\frac{\xi(0)}{2}} := \frac{\xi(0)}{2} - m_0\pi \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$, and $\widetilde{\frac{\xi(\tau)}{2}} := \frac{\xi(\tau)}{2} - (m_0 - m_t)\pi \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$. Then,

$$\begin{aligned}&\int_0^t \frac{1}{L(\tau)^2} d\tau \\ &= \frac{1}{2}(m_t - 1)\pi + \frac{1}{2}\int_{\frac{\xi(0)}{2}}^{m_0\pi+\frac{\pi}{2}} f(\tau)d\tau + \frac{1}{2}\int_{(m_0+m_t)\pi-\frac{\pi}{2}}^{\frac{\xi(0)}{2}+2t} f(\tau)d\tau \\ &= (m_t-1)\frac{\pi}{2} + \frac{1}{2}\int_{\widetilde{\frac{\xi(0)}{2}}}^{\frac{\pi}{2}} f(\tau)d\tau + \frac{1}{2}\int_{-\frac{\pi}{2}}^{\widetilde{\frac{\xi(t)}{2}}} f(\tau)d\tau \\ &= (m_t-1)\frac{\pi}{2} + \frac{1}{2}\left[\arctan\left((c_1+c_2)\tan(\tau)\right)\right]_{\widetilde{\frac{\xi(0)}{2}}}^{\frac{\pi}{2}} + \frac{1}{2}\left[\arctan\left((c_1+c_2)\tan(\tau)\right)\right]_{-\frac{\pi}{2}}^{\widetilde{\frac{\xi(t)}{2}}} \\ &= (m_t-1)\frac{\pi}{2} + \frac{\pi}{2} - \frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\widetilde{\frac{\xi(0)}{2}}\right)\right) \\ &\qquad + \arctan\left((c_1+c_2)\tan\left(\widetilde{\frac{\xi(t)}{2}}\right)\right) + \frac{\pi}{2} \\ &= m_t\frac{\pi}{2} + \frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\widetilde{\frac{\xi(t)}{2}}\right)\right) - \frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\widetilde{\frac{\xi(0)}{2}}\right)\right) \\ &= m_t\frac{\pi}{2} + \frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\frac{\xi(t)}{2}\right)\right) - \frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\frac{\xi(0)}{2}\right)\right).\end{aligned}$$

Hence

$$\begin{aligned}\gamma(t) &= \int_0^t \left[|\beta(\tau)|^2 - |X(\tau)|^2 + \frac{\omega}{L(\tau)^2}\right] d\tau + \gamma(0) \\ &= \gamma(0) + \sum_{l=1}^{d} \frac{a_l}{2}\left[\sin(2\theta_l(t)) - \sin(2\theta_l(0))\right] \\ &\quad + \frac{\omega}{2}\arctan\left((c_1+c_2)\tan\left(\frac{\xi(t)}{2}\right)\right) \\ &\quad - \frac{\omega}{2}\arctan\left((c_1+c_2)\tan\left(\frac{\xi(0)}{2}\right)\right) + m_t\frac{\pi}{2}.\end{aligned}$$

□

Lemma 2 (Action-angle variables from the parameters). *The change of variables* $(L, B, X, \beta) \mapsto (h, a, \xi, \theta)$ *is explicit, and at time* $t = 0$ *we have*

$$\begin{aligned} a_i(0) &= \frac{1}{2}\left(X_i(0)^2 + \beta_i(0)^2\right), \quad i = 1, \dots, d, \\ \theta_i(0) &= \arctan\left(\frac{X_i(0)}{\beta_i(0)}\right), \quad i = 1, \dots, d, \\ h(0) &= \frac{L(0)^4 + 1 + B(0)^2}{4L(0)^2}, \\ \xi(0) &= \arctan\left(\frac{B(0)}{2h(0) - L(0)^2}\right), \end{aligned} \tag{24}$$

whenever $\theta_i(0)$ *and* $\xi(0)$ *are well-defined. When any one of them is ill-defined – which happens when* $X_i(0) = \beta_i(0) = 0, i \in \{1, \dots, d\}$ *or when* $L(0) = 1$ *and* $B(0) = 0$ *– any value can be taken and the time evolution of* $A(t)$*,* $L(t)$*,* $B(t)$*,* $X(t)$*,* $\beta(t)$ *and* $\gamma(t)$ *will not depend on the value. Moreover, in the cases where* $a_i(0) = 0$*,* $i \in \{1, \dots, d\}$ *or* $h(0) = \frac{1}{2}$*, the formula* (24) *for* $\theta_i(0)$*,* $i \in \{1, \dots, d\}$ *or* $\xi(0)$ *are ill-defined, but any value can be taken as a substitution and this will not affect the behavior of the mappings* $t \mapsto \gamma(t)$ *and* $t \mapsto s(t)$*.*

Proof. The proof of this Lemma consists in inverting the expressions (19) using algebraic manipulations. ☐

Let us sum up this section: we have shown that, if the initial condition U_0 to the nonlinear Schrödinger equation can be written as a modulated soliton $U_0 = \mathcal{M}_{P_0}Q$, then it is possible to write the time-dependent solution $u(t)$ as a modulated soliton. In other words, $u(t,x) = (\mathcal{M}_{P(t)}Q)(t,x)$. Since the time-dependence is now only through the parameters P, we write $u(t,x) = (\mathcal{M}_{P(t)}Q)(x)$. The time-dependent modulation parameters involved in $\mathcal{M}_{P(t)}$ are known exactly for all times t by Lemma 1.

3. Two or more solitons

3.1. *Modulated solitons manifold*

Assume now that the initial condition U_0 is a sum of N solitons

$$U_0 = \sum_{n=1}^{N} u^n := \sum_{n=1}^{N} \mathcal{M}_{P_0^n} v^n,$$

where P_0^n are the initial modulation parameters associated to the n-th function v^n. We recall that the superscript is not meant as an exponent here.

Even though the computation of the nonlinearity $u|u|^2$ involves the interaction of all triplets of solitons, the most important interaction for each soliton will be the self-interaction. In this section we will show that the nonlinear Schrödinger equation involving u can be split into N nonlinear Schrödinger equations involving u^n, up to some generally less important interaction terms. We can then solve each nonlinear Schrödinger equation on u^n using Section 2.2, and the remaining interaction terms can be approximated numerically using a procedure based on the Dirac-Frenkel principle.

We focus now on (2) in the case of modulating soliton. It means that we search an approximation

$$u(t,x) \approx \sum_{j=1}^{N} u^j(t,x) := \sum_{j=1}^{N} \frac{\exp\left\{ i\gamma^j + iL^j\beta^j \cdot y^j + i\frac{B^j}{2}|y^j|^2 \right\}}{(L^j)^{d/2}} Q_j(y^j), \tag{25}$$

where all the parameters are time-dependent, and where Q^j are solitons solutions of (4) with possible different frequencies ω_j. For simplicity, we will assume in the following that all solitons are associated to the same eigenvalue ω, *i.e.* that we have $Q^j = Q$ for all j, where Q is a given solution of (4).

Remark 1. We do not address here the problem of general approximaton of any function by a sum of modulated solitons. Here, we assume that the initial datum is under this form, which is relevant in many physical applications, see for instance [9, 35] and the references therein.

The numerical method we are looking for aims at approximating the time evolution of all the parameters while keeping the modulation ansatz. This naturally calls for the Dirac-Frenkel principle. Let $\mathcal{V}$ be the modulation manifold defined by

$$\mathcal{V} := \left\{ u \in L^2(\mathbb{R}^d) \;\middle|\; \begin{array}{c} u(x) = \displaystyle\sum_{j=1}^{N} (\mathcal{M}_{P^j} Q)(x) \in L^2(\mathbb{R}^d) \\ P^j = (\gamma^j, X^j, \beta^j, B^j, L^j) \in \mathbb{R}^{2d+2} \times \mathbb{R}_+,\ 1 \le j \le N \end{array} \right\}.$$

Let $\mathcal{T}_{u(t)}\mathcal{V}$ be the tangent space at $u(t)$ of $\mathcal{V}$ viewed as a real submanifold of L^2 (itself viewed as a real Hilbert space associated with the scalar product

$\langle\,\cdot\,,\,\cdot\,\rangle$ defined by (7)). Note that any point on the manifold $\mathcal{V}$ can be parametrized by the coordinate vector

$$P := \{P^1, \dots, P^N\},$$

and if we write $u(x) = u_P(x)$, the projection of (1) on the manifold can be written (through the Dirac-Frenkel principle) for $u(t,x) = u_{P(t)}(x)$:

$$\forall\, f \in T_{u(t)}\mathcal{V} \quad \langle f, \partial_t u - i\Delta u + i|x|^2 u + i\mu|u|^2 u\rangle = 0.$$

By taking a local basis of $\mathcal{T}_{u(t)}\mathcal{V}$, this equation can be recast as a nonlinear system of ordinary differential equation on P, of the form

$$B(P)\dot{P} = F(P)$$

where $B(P)$ is a matrix and $F(P)$ a vector field. The exact expression of P will be revealed later, but first we propose a natural splitting of the vector field which takes advantage of the structure of the soliton.

3.2. *Splitting of the equation*

The vector field $F(P)$ can be decomposed according to the structure of $u = \sum_j u^j$. Let us compute $|u|^2 u$:

$$\begin{aligned} \left|\sum u^j\right|^2 \sum u^j &= \left(\sum_j u^j\right)\left(\sum_k \overline{u^k}\right)\sum_l u^l = \sum_{j,k,l} u^j \overline{u^k} u^l \\ &= \sum_{j=1}^N |u^j|^2 u^j + \sum_{j=1}^N \sum_{(k,l)\neq(j,j)} u^j \overline{u^k} u^l. \end{aligned}$$

Hence we can write

$$B(P)\dot{P} = F(P) = F_1(P) + F_2(P) \tag{26}$$

where F_1 corresponds to the part

$$i\partial_t u = -\Delta_x \sum_{j=1}^N u^j + |x|^2 \sum_{j=1}^N u^j + \mu \sum_{j=1}^N |u^j|^2 u^j, \tag{F1}$$

which is the *soliton* part, and F_2 the remainder term corresponding to the equation

$$i\partial_t u = \mu \sum_j \sum_{(k,l)\neq(j,j)} u^j \overline{u^k} u^l \tag{F2}$$

projected onto the manifold $\mathcal{V}$, which is the *interactions* part.

Note that when the solitons are rather localized and their centers X^k are all far from each other, we expect the interaction terms to be small: $\sum_{j=1}^N \sum_{(k,l)\neq(j,j)} u^j \overline{u^k} u^l \ll 1$ (typically exponentially decreasing with respect to the distance between the solitons).

Now, the content of Section 2.2 precisely shows that the (F1) equation can be solved exactly on the manifold $\mathcal{V}$ by choosing $u^j = \mathcal{M}_{P^j} Q$, separately solving the equation

$$\forall\, j = 1, \dots, N, \quad i\partial_t u^j + \Delta_x u^j - |x|^2 u^j = \mu |u^j|^2 u^j, \tag{27}$$

through the modulation equations described in Section 2.4.

Hence we only need to project the equation (F2) onto the manifold $\mathcal{V}$ to obtain a natural splitting of the equation (26). The Dirac-Frenkel principle applied to (F2) consists in looking for solutions to

$$\left| \begin{array}{l} \text{Find } \partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{V}, \text{ such that} \\ \qquad \left\langle f, i\partial_t \sum_{j=1}^N u^j - \mu \sum_{j=1}^N \sum_{\substack{k,l=1 \\ (k,l)\neq(j,j)}}^N u^j \overline{u^k} u^l \right\rangle = 0, \qquad \forall f \in \mathcal{T}_{u(t)}\mathcal{V}. \end{array} \right. \tag{28}$$

Let $S_{u(t)}$ be a basis of $\mathcal{T}_{u(t)}\mathcal{V}$, then (28) is equivalent to

$$\left| \begin{array}{l} \text{Find } \partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{V}, \text{ such that} \\ \qquad \left\langle f, i\partial_t \sum_{j=1}^N u^j \right\rangle = \mu \left\langle f, \sum_{j=1}^N \sum_{\substack{k,l=1 \\ (k,l)\neq(j,j)}}^N u^j \overline{u^k} u^l \right\rangle, \forall f \in S_{u(t)}. \end{array} \right. \tag{29}$$

A family (which may happen to be linearly dependent) spanning the tangent space $\mathcal{T}_{u(t)}\mathcal{V}$ is given by

$$\begin{aligned} S_{u(t)} &= \left\{ \begin{array}{c} e^{i\Gamma^j(y^j)} Q(y^j), (y_1^j) e^{i\Gamma^j(y^j)} Q(y^j), \dots, (y_d^j) e^{i\Gamma^j(y^j)} Q(y^j), \\ i e^{i\Gamma^j(y^j)} \partial_{y_1} Q(y^j), \dots, i e^{i\Gamma^j(y^j)} \partial_{y_d} Q(y^j), |y^j|^2 e^{i\Gamma^j(y^j)} Q(y^j), \\ i e^{i\Gamma^j(y^j)} \left(\frac{d}{2} + y \cdot \nabla \right) Q(y^j) \end{array} \right\}_{j=1}^N \\ &=: \left\{ b_0^j, \dots, b_{2d+2}^j : j = 1, \dots, N \right\}, \end{aligned} \tag{30}$$

where we defined

$$\Gamma^j(y^j) := \gamma^j + L^j \beta^j \cdot y^j + \frac{B^j}{2} |y^j|^2.$$

This family $S_{u(t)}$ indeed spans the tangent space $\mathcal{T}_{u(t)}\mathcal{V}$ because $\partial_t u$ writes as a linear combination of all the b_q^p, by (14). We can rewrite (29) as

$$\left|\begin{array}{l}\text{Find } \partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{V}, \text{ such that for } p \in [\![1,N]\!], q \in [\![0,2d+2]\!]. \\ \qquad \left\langle b_q^p, i\partial_t \sum_{j=1}^{N} u^j \right\rangle = \mu \left\langle b_q^p, \sum_{\substack{j,k,l=1 \\ (k,l)\neq(j,j)}}^{N} u^j \overline{u^k} u^l \right\rangle .\end{array}\right. \tag{31}$$

The next step consists in expressing (31) as a linear system involving the modulation parameters and their time derivative, which will yield ordinary differential equations that can be integrated numerically.

For $u \in \mathcal{V}$, we can write (14) in a more convenient form:

$$\begin{aligned} i\partial_t u &= \sum_{j=1}^{N} \left(b_0^j, \dots, b_{2d+2}^j\right) \underbrace{\frac{1}{(L^j)^{d/2}} \begin{pmatrix} -\dot\gamma^j + \beta^j \cdot \dot X^j \\ -L^j \dot\beta_1^j + \frac{B^j}{L^j}\dot X_1^j \\ \vdots \\ -L^j \dot\beta_d^j + \frac{B^j}{L^j}\dot X_d^j \\ -\frac{\dot X_1^j}{L^j} \\ \vdots \\ -\frac{\dot X_d^j}{L^j} \\ \frac{B^j \dot L^j}{L^j} - \frac{\dot B^j}{2} \\ -\frac{\dot L^j}{L^j} \end{pmatrix}}_{=:D^j} \\ &= \left(b_0^1, \dots, b_{2d+2}^1, b_0^2, \dots, b_{2d+2}^N\right) \begin{pmatrix} D^1 \\ \vdots \\ D^N \end{pmatrix}. \end{aligned}$$

We are now able to rewrite (31) under matrix form

$$\mathbf{A}D = S, \tag{32}$$

where $\mathbf{A} \in \mathbb{C}^{(2d+3)N\times(2d+3)N}$ is the projection matrix, $D \in \mathbb{R}^{(2d+3)N}$ is a vector containing the modulation parameters and their derivative, and $S \in \mathbb{C}^{(2d+3)N}$ contains the projection of the nonself-interactions. More precisely,

$$D = \begin{pmatrix} D^1 \\ \vdots \\ D^N \end{pmatrix} \tag{33}$$

with $D^j \in \mathbb{R}^{2d+3}$,

$$\mathbf{A} = \begin{pmatrix} \langle b_0^1, b_0^1, \rangle & \dots & \langle b_0^1, b_{2d+2}^1 \rangle & \langle b_0^1, b_0^2 \rangle & \dots & \langle b_0^1, b_{2d+2}^N \rangle \\ \vdots & & \vdots & \vdots & & \vdots \\ \langle b_{2d+2}^N, b_0^1, \rangle & \dots & \langle b_{2d+2}^N, b_{2d+2}^1 \rangle & \langle b_{2d+2}^N, b_0^2 \rangle & \dots & \langle b_{2d+2}^N, b_{2d+2}^N \rangle \end{pmatrix}, \tag{34}$$

and

$$S = \mu \begin{pmatrix} \left\langle b_0^1, \sum_{j=1}^N \sum_{\substack{k,l=1 \\ (k,l)\neq(j,j)}}^N u^j \overline{u^k} u^l \right\rangle \\ \vdots \\ \left\langle b_{2d+2}^N, \sum_{j=1}^N \sum_{\substack{k,l=1 \\ (k,l)\neq(j,j)}}^N u^j \overline{u^k} u^l \right\rangle \end{pmatrix}. \tag{35}$$

It will be convenient later to write $D^j = \mathbf{C}^j \dot{P}^j$, where

$$P^j = \left(\gamma^j, X_1^j, \dots, X_d^j, \beta_1^j, \dots, \beta_d^j, B^j, L^j\right), \tag{36}$$

and

$$\mathbf{C}^j = \begin{pmatrix} -1 & \beta_1^j & \dots & \beta_d^j & 0 & \dots & 0 & 0 & 0 \\ 0 & \frac{B^j}{L} & & 0 & -L^j & & 0 & 0 & 0 \\ \vdots & & \ddots & & & \ddots & & \vdots & \vdots \\ 0 & 0 & & \frac{B^j}{L} & 0 & & -L^j & 0 & 0 \\ 0 & -\frac{1}{L^j} & & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & & \ddots & & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & & -\frac{1}{L^j} & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 & -\frac{1}{2} & \frac{B^j}{L^j} \\ 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & -\frac{1}{L^j} \end{pmatrix} \in \mathbb{C}^{(2d+3)\times(2d+3)}. \tag{37}$$

It is readily seen that $\mathbf{C}$ is invertible for $L \neq 0$.

Once the linear system (32) is solved, we obtain the solution vector D, from which we can update the modulation parameters. In order to solve numerically the linear system, we rewrite it to use only real matrices. Let $\mathbf{A}_\Re := \Re(\mathbf{A})$, $\mathbf{A}_\Im := \Im(\mathbf{A})$, $D_\Re := \Re(D)$, $D_\Im := \Im(D)$, $S_\Re := \Re(S)$, and $S_\Im := \Im(S)$.

$$\begin{aligned} \mathbf{A}D = S &\iff (\mathbf{A}_\Re + i\mathbf{A}_\Im)(D_\Re + iD_\Im) = S_\Re + iS_\Im \\ &\iff \begin{cases} \mathbf{A}_\Re D_\Re - \mathbf{A}_\Im D_\Im = S_\Re \\ \mathbf{A}_\Im D_\Re + \mathbf{A}_\Re D_\Im = S_\Im \end{cases} \\ &\iff \begin{pmatrix} \mathbf{A}_\Re & -\mathbf{A}_\Im \\ \mathbf{A}_\Im & \mathbf{A}_\Re \end{pmatrix} \begin{pmatrix} D_\Re \\ D_\Im \end{pmatrix} = \begin{pmatrix} S_\Re \\ S_\Im \end{pmatrix}. \end{aligned} \tag{38}$$

It is more convenient to solve (38) than (32), because we only have to deal with real matrices and vectors. Once (38) is solved, we obtain (33), where each D^j is given by

$$D^j = \begin{pmatrix} -\dot{\gamma}^j + \beta^j \cdot \dot{X}^j \\ -L^j \dot{\beta}_1^j + \frac{B^j}{L^j}\dot{X}_1^j \\ \vdots \\ -L^j \dot{\beta}_d^j + \frac{B^j}{L^j}\dot{X}_d^j \\ -i\frac{\dot{X}_1^j}{L^j} \\ \vdots \\ -i\frac{\dot{X}_d^j}{L^j} \\ \frac{B^j \dot{L}^j}{L^j} - \frac{\dot{B}^j}{2} \\ -i\frac{\dot{L}^j}{L^j} \end{pmatrix} = (L^j)^{d/2}\left(D_{\Re}^j + iD_{\Im}^j\right).$$

Since D^j is a real vector, we get

$$D^j = \mathbf{C}^j \dot{P}^j = (L^j)^{d/2} D_{\Re}^j \qquad \Longleftrightarrow \qquad \dot{P}^j = (\mathbf{C}^j)^{-1}(L^j)^{d/2} D_{\Re}^j. \tag{39}$$

The imaginary part $D_{\Im}^j$ is discarded due to the approximation made by the Dirac-Frenkel principle. The combination of (38) and (39) corresponds to the F_2 part of the system (26). Note that this part is a highly nonlinear system in terms of P, as all the terms in the matrices depend on P. Moreover, the interaction term S defined in (35) has to be implemented numerically.

3.3. *Computing interactions numerically*

3.3.1. *Numerical approximation of solitons*

In the ansatz (25) we need to be able to compute the soliton Q numerically. To do this, we use the classical Normalized Gradient method (see [36] and the references therein), which gives an approximation of the soliton on a numerical grid. Let us recall that it consists in approximating the solution of (4) by a combination of the discretization of the parabolic equation

$$\left| \begin{aligned} &\partial_t \psi = (\Delta - |x|^2)\psi - \mu|\psi|^2\psi \\ &\psi(n\tau) = \psi_n \end{aligned} \right. \tag{40}$$

on a small time interval $[n\tau, (n+1)\tau]$ and a renormalization step $\psi_n \mapsto \frac{\psi_n}{\|\psi_n\|_{L^2}}$, for $n = 1, 2, \ldots$. The discretization of the parabolic equation (40) is usually done using the implicit Euler scheme, and the global scheme is expected to converge towards the solution of (4) of minimal energy and L^2 norm 1 (the ground state, radially symmetric and decreasing with respect to the radius) as proved in [36] in the 1D case. Note that we can easily adapt this algorithm to obtain a soliton of any norm. We can also adapt this algorithm to solitons with specific rotational symmetries to obtain other type of solutions to (4).

In the numerical examples below, we choose a finite-size grid, with N nodes along each dimension, and perform the Normalized Gradient method on this grid. We can use a Discrete Fourier transform to have a better computation of the Laplacian than finite differences. We can also seek solitons Q with specific rotational symmetries in 2D and write the equation in polar coordinates, but the grid matching between solitons is slightly more complicated to implement. Once the approximation $\widetilde{Q}$ of the exact soliton Q is obtained on this grid, it is extended by zero outside of the grid and interpolated using periodic cubic splines to have a continuous representation of the soliton approximation. The derivatives of $\widetilde{Q}$ are approximated using a pseudo-spectral method – in this case the Fourier transform, via the Fast Fourier Transform – extended by zero outside the grid, and interpolated using periodic cubic splines.

Note that the Normalized Gradient method can be performed as part of a pre-computation step, and only the values of the soliton on the grid need to be saved. This pre-computation will be done in our numerical experiments to avoid the consequent overhead of computing the soliton values on a fine grid.

3.3.2. *Interaction grids*

In (34) and (35), we need to compute $L^2(\mathbb{R}^d)$ inner product between solitons centered at possibly different locations. The L^2 inner product $\langle f, g\rangle$ can be approximated using a grid if both functions f and g are known on this grid. If it is not the case – and it is in practice never the case as the translation vector X^j are arbitrary – we have to somehow get an approximation of the two functions on the same grid.

We have chosen to first obtain f and g on a grid, and then perform a linear interpolation of both functions. They are extended by zero outside of their respective grids, and this allows us to compute efficiently the inner product by only approximating the integral on a region that is common to both grids.

3.3.3. *Time integration*

In the integration of the system (26), we have seen that we can integrate the $F_1(P)$ part exactly. The interaction part $F_2(P)$ obtained by the Dirac-Frenkel principle are then integrated numerically using the midpoint formula (see for instance [28]).

3.3.4. *Detailed algorithm*

Algorithm 1 Modulation based algorithm with Strang splitting

```
Require:
    • $M$: number of discretization points for each dimension
    • $x_{\min}, x_{\min}$: the grid on which to look for an approximation of the soliton is $[x_{\min}, x_{\max}]^d$
    • $N$: number of modulated solitons in the ansatz
    • $L^j, X^j, \beta^j, B^j, \gamma^j$ for $j = 1, \dots, N$: initial parameters of each modulated soliton
    • $\Delta t, T$: stepsize and final time of the simulation
    • $\eta$: numerical tolerance
  Apply the Normalized Gradient method to obtain an approximation of $Q$ on $[x_{\min}, x_{\max}]^d$ using $M$ points for each dimension and a tolerance $\eta$.
  Interpolate the values on the grid, and extend it by zero outside the grid.
  for $t = \Delta t, 2\Delta t, \dots, T$ do
      Update the modulation parameters on a timestep $\frac{\Delta t}{2}$ using Lemma 1
      Use the Dirac-Frenkel equations (38)-(39) to approximate the time evolution of the modulation parameters, over a timestep $\Delta t$
      Update the modulation parameters on a timestep $\frac{\Delta t}{2}$ using Lemma 1
  end for
```

3.4. ***Study of error with a single modulated soliton***

We show that the scheme presented above yields a good approximation of the true solution, in the simple case of a single soliton. In this situation, the parameters are given for all times by Lemma 1 since the Dirac-Frenkel principle has right-hand side $S = 0$.

Let us resume our setting: we are looking for a solution

$$u(t, x) = (\mathcal{M}_{P(t)} Q)(x)$$

to (1) but in practice, we cannot know Q exactly and we can only approximate it on a grid. For simplicity, let us assume this grid to be defined as follows: let $G = [-\alpha, \alpha]^2$ for some $\alpha > 0$, and write $G_{\Delta x}$ its discretization using a uniform stepsize $\Delta x > 0$. Using the Normalized Gradient method to approximate Q on the grid $G_{\Delta x}$, we obtain the approximate solution

$$\widetilde{u}(t,x) = (\mathcal{M}_{P(t)}\widetilde{Q})(x),$$

where $\|Q - \widetilde{Q}\|_{L^2(G_{\Delta x})} \leq \eta$, and we extend $\widetilde{Q}$ by interpolation on the full box G, and by zero on $\mathbb{R}^2 \setminus G$. The gradient $\nabla\widetilde{Q}$ is assumed to be computed on $G_{\Delta x}$ with a pointwise error of order $\mathcal{O}(\Delta x^\sigma)$ for some $\sigma > 0$ (e.g. $\sigma = 1$ for finite differences of order 1).

Lemma 3 (Normalized Gradient method estimates). *Let* $\varepsilon_p(\alpha) := \|Q|y|^p\|^2_{L^2(\mathbb{R}^2\setminus G)}$ *and* $\epsilon(\alpha) := \|\nabla Q\|^2_{L^2(\mathbb{R}^2\setminus G)}$. *We have the following estimates:*

$$\|Q - \widetilde{Q}\|_{L^2(\mathbb{R}^2)} \lesssim \sqrt{\eta^2 + (\alpha\Delta x)^2 + \varepsilon_0(\alpha)},$$

$$\|(Q - \widetilde{Q})\nabla M\|_{L^2(\mathbb{R}^2)} \lesssim \sqrt{(1 + |\alpha|^2)\left(\eta^2 + (\alpha\Delta x)^2\right) + \varepsilon_1(\alpha)},$$

$$\|M\nabla(Q - \widetilde{Q})\|_{L^2(\mathbb{R}^2)} \lesssim \sqrt{\alpha^2(\Delta x)^\sigma + C'(\alpha\Delta x)^2 + \epsilon(\alpha)},$$

where the implicit constants depend on the modulation parameters at time $t = 0$ *as well as on*

$$\|\nabla Q\|_{L^\infty}, \quad \|\nabla^2 Q\|_{L^\infty}, \quad \|\nabla\widetilde{Q}\|_{L^\infty}, \quad \textit{and} \quad \|\nabla^2\widetilde{Q}\|_{L^\infty},$$

that are assumed to be bounded independently on Δx, α *and* η.

Proof. By a Taylor-Lagrange expansion, for $x \in [-\Delta x, \Delta x]^2$, there exist $\theta, \widetilde{\theta} \in (-\Delta x, \Delta x)$ such that

$$Q(x) - \widetilde{Q}(x) = Q(0) + x \cdot \nabla Q(\theta) - \left(\widetilde{Q}(0) + x \cdot \nabla\widetilde{Q}(\widetilde{\theta})\right).$$

We get

$$\begin{aligned}
&\int_{[-\Delta x,\Delta x]^2} \left|Q(x) - \widetilde{Q}(x)\right|^2 dx \\
&= \int_{[-\Delta x,\Delta x]^2} \left|Q(0) + x \cdot \nabla Q(\theta) - \left(\widetilde{Q}(0) + x \cdot \nabla\widetilde{Q}(\widetilde{\theta})\right)\right|^2 dx \\
&\leq 2\int_{[-\Delta x,\Delta x]^2} \left|Q(0) - \widetilde{Q}(0)\right|^2 dx + 2\int_{[-\Delta x,\Delta x]^2} \left|x \cdot \nabla Q(\theta) - x \cdot \nabla\widetilde{Q}(\widetilde{\theta})\right|^2 dx \\
&\leq 2\int_{[-\Delta x,\Delta x]^2} \left|Q(0) - \widetilde{Q}(0)\right|^2 dx + 2\int_{[-\Delta x,\Delta x]^2} |x|^2 \left|\nabla Q(\theta) - \nabla\widetilde{Q}(\widetilde{\theta})\right|^2 dx \\
&\leq 2(\Delta x)^2 \left|Q(0) - \widetilde{Q}(0)\right|^2 + 4C(\Delta x)^4,
\end{aligned}$$

where C depends on L^∞ on ∇Q and $\nabla\widetilde{Q}$. Then, similarly

$$\begin{aligned}
\|Q-\widetilde{Q}\|^2_{L^2(G)} &= \int_G \left|Q-\widetilde{Q}\right|^2 dx \\
&= \sum_{g\in G_{\Delta x}} \int_{g_1}^{g_1+\Delta x}\int_{g_2}^{g_2+\Delta x} \left|Q(x)-\widetilde{Q}(x)\right|^2 dx \\
&\le 2(\Delta x)^2 \sum_{g\in G_{\Delta x}} \left|Q(g)-\widetilde{Q}(g)\right|^2 + 4C\sum_{g\in G}(\Delta x)^4 \\
&\lesssim \|Q-\widetilde{Q}\|^2_{L^2(G_{\Delta x})} + C\alpha^2(\Delta x)^2 \lesssim \eta^2 + C\alpha^2(\Delta x)^2. \qquad (41)
\end{aligned}$$

We recall that $\widetilde{Q}$ is extended by zero on $\mathbb{R}^2\setminus G$, which shows the first estimate.

For the second estimate, we have

$$\begin{aligned}
&\left\|(Q-\widetilde{Q})\nabla M\right\|^2_{L^2(\mathbb{R}^2)} = \left\|(Q-\widetilde{Q})(L\beta+By)M\right\|^2_{L^2(\mathbb{R}^2)} \\
&= \left\|(Q-\widetilde{Q})\left(\beta+\frac{B}{L}y\right)\right\|^2_{L^2(\mathbb{R}^2)} \\
&\le 2\left(|\beta|^2+2\left|\frac{B}{L}\alpha\right|^2\right)\left\|Q-\widetilde{Q}\right\|^2_{L^2(G)} + \left\|(Q-\widetilde{Q})\left(\beta+\frac{B}{L}y\right)\right\|^2_{L^2(\mathbb{R}^2\setminus G)}.
\end{aligned}$$

By Lemma 1, there exists $C_1 = C(\beta(0), L(0), B(0))$ such that

$$\left\|(Q-\widetilde{Q})\nabla M\right\|^2_{L^2(\mathbb{R}^2)} \le 2C_1\left(1+|\alpha|^2\right)\left\|Q-\widetilde{Q}\right\|^2_{L^2(G)} + C_1\|Qy\|^2_{L^2(\mathbb{R}^2\setminus G)},$$

and we conclude using (41). The third estimate is obtained in a similar fashion:

$$\begin{aligned}
\left\|M\nabla(Q-\widetilde{Q})\right\|^2_{L^2(\mathbb{R}^2)} &= \left\|\nabla_y(Q-\widetilde{Q})\right\|^2_{L^2(G)} + \epsilon(\alpha) \\
&\lesssim \left\|\nabla_y(Q-\widetilde{Q})\right\|^2_{L^2(G_{\Delta x})} + C'(\Delta x)^2\alpha^2 + \epsilon(\alpha),
\end{aligned}$$

where C' depends on L^∞ bounds on the Hessian matrices of Q and $\widetilde{Q}$. Owing to the pointwise error estimate on the gradients we get

$$\left\|M\nabla(Q-\widetilde{Q})\right\|^2_{L^2(\mathbb{R}^2)} \lesssim \alpha^2(\Delta x)^\sigma + (\alpha\Delta x)^2 + \epsilon(\alpha),$$

which achieves the proof. □

Proposition 2. *The following estimates hold:*

$$\|u-\widetilde{u}\|_{L^2(\mathbb{R}^2)} \lesssim \sqrt{\eta^2+(\Delta x)^2\alpha+\varepsilon(\alpha)},$$

and

$$\begin{aligned}
\|\nabla u-\nabla\widetilde{u}\|_{L^2(\mathbb{R}^2)} \lesssim&\sqrt{\left(1+|\alpha|^2\right)\left(\eta^2+(\alpha\Delta x)^2\right)+\varepsilon_1(\alpha)} \\
&+\sqrt{\alpha^2(\Delta x)^\sigma + C'(\alpha\Delta x)^2+\epsilon(\alpha)}.
\end{aligned}$$

Proof. By a change of variables,

$$\|\widetilde{u}\|_{L^2(\mathbb{R}^2)}^2 = \int_{\mathbb{R}^2} \left| \frac{1}{L} e^{i\gamma + iL\beta\cdot y(t,x) + \frac{iB}{2}|y(t,x)|^2} \widetilde{Q}(y(t,x)) \right|^2 dx = \int_{\mathbb{R}^2} \left| \widetilde{Q}(y) \right|^2 dy,$$

which is time-independent. For the L^2 norm estimate of $u - \widetilde{u}$,

$$\begin{aligned} \|u - \widetilde{u}\|_{L^2(\mathbb{R}^2)}^2 &= \frac{1}{L^2} \|Q \circ y - \widetilde{Q} \circ y\|_{L^2(\mathbb{R}^d)}^2 = \|Q - \widetilde{Q}\|_{L^2(\mathbb{R}^d)}^2 \\ &\lesssim \eta^2 + (\alpha \Delta x)^2 + \varepsilon(\alpha). \end{aligned}$$

For the gradient of the difference,

$$\begin{aligned} &\|\nabla u - \nabla \widetilde{u}\|_{L^2(\mathbb{R}^2)} \\ &= \left\| Q \circ y \nabla_x M + M \nabla_x Q \circ y - \widetilde{Q} \circ y \nabla_x M - M \nabla_x \widetilde{Q} \circ y \right\|_{L^2(\mathbb{R}^2)} \\ &= \frac{1}{L} \left\| Q \circ y \nabla_y M + M \nabla_y Q \circ y - \widetilde{Q} \circ y \nabla_y M - M \nabla_y \widetilde{Q} \circ y \right\|_{L^2(\mathbb{R}^2)} \\ &= \left\| Q \nabla M + M \nabla Q - \widetilde{Q} \nabla M - M \nabla \widetilde{Q} \right\|_{L^2(\mathbb{R}^2)} \\ &\leq \left\| Q \nabla M - \widetilde{Q} \nabla M \right\|_{L^2(\mathbb{R}^2)} + \left\| M \nabla Q - M \nabla \widetilde{Q} \right\|_{L^2(\mathbb{R}^2)}. \end{aligned}$$

We get the claimed estimate by using Lemma 3. ☐

4. Numerical results

The efficiency of the proposed method is assessed based on the relative evolution of conservative quantities. For a quantity $q(t)$, its relative evolution is defined as

$$q_{\mathrm{rel}}(t) := \frac{q(t) - q(0)}{q(0)}, \quad t \geq 0.$$

The numerical simulations are all done over a time interval $[0, T]$, $T = 100$, discretized with a stepsize $\Delta t = 10^{-1}$.

For the soliton approximation, we have chosen a grid of $M = 100$ points in each direction, and looked for the soliton approximation over $[-5, 5] \times [-5, 5]$. The Normalized Gradient method is applied until two successive iterations ψ_n and ψ_{n+1} satisfy $\|\psi_n - \psi_{n+1}\|_{L^2} \leq \eta = 10^{-9}$.

For the computation of the conservative quantities, we approximate the first-order derivatives of the soliton using the Discrete Fourier method – in practice, using the FFT – and the derivatives of $M_{P(t)}(x)$ are computed exactly.

The results are not compared with those of a grid-based method, because it is not known beforehand what size should the grid be: even if $X(0) = (0, 0)$, if $\beta(0) = (a, a)$ for a large then the soliton will move far away from the origin. A purely grid-based method has no means of knowing what size the grid should be only based on the initial condition. The same holds for the stepsize of the grid: the grid has to account for the fast variations of the solutions, but it cannot know the fastest variations the solution will have at any time $t > 0$ only based on the initial condition.

4.1. *A single moving soliton*

The initial condition is made of a single modulated soliton, with parameters $X(0) = (5, 0)$, $\beta(0) = (0, 2)$, $L(0) = 1.5$, $B(0) = 0$, $\gamma(0) = 0$. The nonlinearity parameter is $\mu = 1$.

For this situation, we expect the algorithm to have excellent performances: the Dirac-Frenkel splitting step has right-hand side $S = 0$ so the approximate parameter derivatives will be zero, and thus the time evolution of the soliton is performed exactly. The numerical results are given in Figure 1.

However, we note that the conservative quantities are not preserved up to machine precision. This is due to the fact that in our implementation, the stepsize δx of the grid used to compute the conservative quantities is chosen to be constant and equal to the stepsize Δx of the grid used for the Normalized Gradient method. In the case of a single soliton, a better choice would be to use $\delta x = L\Delta x$, so that the computation of the conservative quantities would simply be a scaling of the initial condition. Numerical results – not reported here – showed that with this better choice of δx, the conservation is of order 10^{-12} for the L^2 norm and of order 10^{-10} for the energy and momentum. However this perfect choice of δx is not applicable in the general setting of several solitons, and in this case the most natural stepsize is $\delta x = \Delta x$. This explains why the conservative quantities in Figure 1 are not preserved down to machine precision.

4.2. *Rotating solitons*

The initial condition is made of two modulated solitons, one rotating clockwise close to the origin and one rotating anti-clockwise far from the origin.

The nonlinearity parameter is $\mu = 1$, and the initial modulations pa-

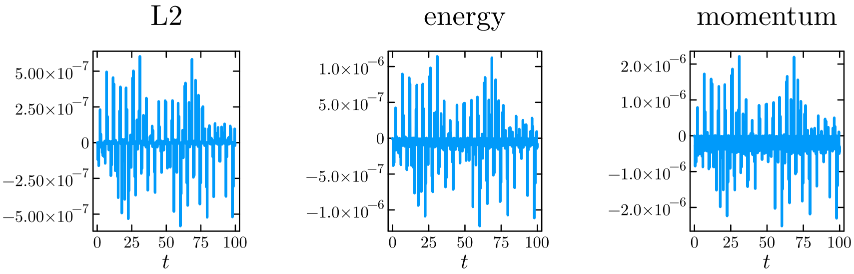

Fig. 1.: Time evolution of the relative conservative quantities: L^2 norm (left), energy (center) and momentum (right), for the single modulated soliton. Nonlinearity parameter $\mu = 1$.

rameters are

$$\begin{array}{lllll} L^1 = 1 & B^1 = 0 & \gamma^1 = 0 & X^1 = (2,-2) & \beta^1 = (X^1)^\perp, \\ L^2 = 0.7 & B^2 = 0 & \gamma^2 = 0 & X^2 = (-4,4) & \beta^2 = (X^2)^\perp, \end{array}$$

where $(x_1, x_2)^\perp = (-x_2, x_1)$, and $\mu = 1$. The parameters are chosen so that the two modulated solitons only interact weakly: weak interactions when $\mu = 1$ mean that the numerical grids associated to u^1 and u^2 have small overlaps. The results are given in Figure 2. Because of the weak interactions, the approximation due to the Dirac-Frenkel principle is small and we can have good conservation properties.

Also, a visual representation of the approximate solution at different times is given in Figure 3.

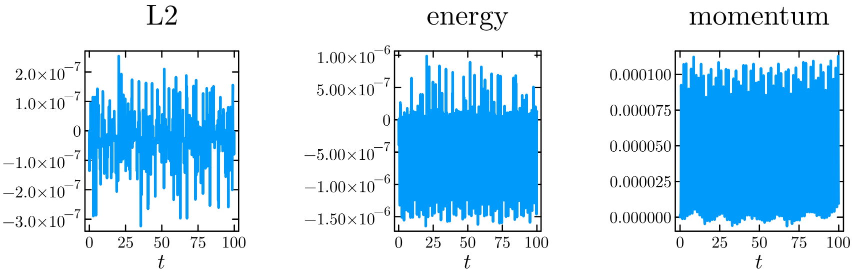

Fig. 2.: Time evolution of the relative conservative quantities: L^2 norm (left), energy (center) and momentum (right), for the two modulated solitons with weak interactions. Nonlinearity parameter $\mu = 1$.

4.3. *Bad scenario*

The third example consists in two solitons interacting heavily. The initial parameters are

$$\begin{array}{lllll} L^1 = 1 & B^1 = 0 & \gamma^1 = 0 & X^1 = (2, -2) & \beta^1 = (X^1)^\perp, \\ L^2 = 0.7 & B^2 = 0 & \gamma^2 = 0 & X^2 = (-4, 4) & \beta^2 = (X^2)^\perp, \end{array}$$

where $(x_1, x_2)^\perp = (-x_2, x_1)$, and they are chosen so that the grids associated to the two modulated solitons have significant overlaps.

We give in Figure 4 the results obtained with a nonlinearity parameter $\mu = 1$, and in Figure 5 the results obtained with a nonlinearity parameter $\mu = 10^{-3}$.

Because of the large overlaps of the two grids, the approximation error due to the Dirac-Frenkel principle – which imposes the ansatz (25) – is large when $\mu = 1$, and thus the numerical solution is a poor approximation of the true solution. The very rough approximations we make in this case can be seen on the relative time evolution of the monitored quantities, and in particular with the energy and momentum. When $\mu = 10^{-3}$, the nonlinearity is smaller and thus the true solution is closer to the ansatz (25), which means the approximation error due to the Dirac-Frenkel principle is smaller. These results underline that the method presented is a good choice in the case of weakly interacting solitons.

5. Conclusion

The goal of this work was to use the theoretical idea of solution modulation for deriving a numerical algorithm.

When a single soliton is considered the modulation parameters are known exactly for all times, and the approximate numerical solution is very close to the true solution – up to some error that depends on the numerical parameters. Moreover the conservative quantities are very well-preserved for the approximate solution, and it is illustrated on a numerical example.

When more than one soliton is considered, we are interested in keeping the ansatz that describes the approximate solution as a sum of modulated solitons, using the Dirac-Frenkel principle. If the modulated solitons only have weak interactions – either they are far from each other or the nonlinearity parameter is small – the approximation error due to the Dirac-Frenkel principle is small and the conservative quantities of the approximate solution are still preserved up to a satisfying error. However, if the solitons interact heavily – either they are close to each other or the nonlinearity parameter is large – the error of the Dirac-Frenkel principle is large and a lot of information is lost during the projection step. Therefore, the conservative quantities of the approximate solution in this case are very poorly preserved.

By studying the error of the approximate soliton obtained via the Normalized Gradient method, we got an estimate on the error of the approximate solution. However, this is done only in the case of a single soliton, because when several solitons are interacting one has to study the error made by the Dirac-Frenkel principle.

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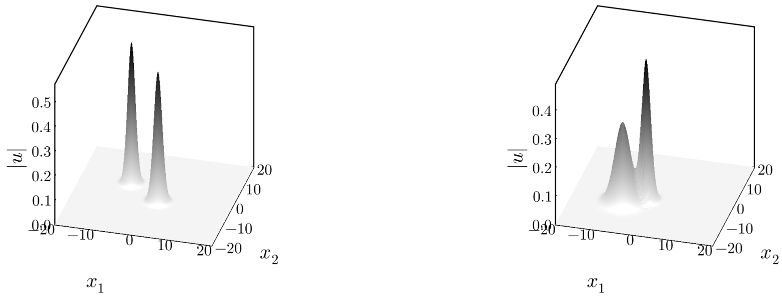
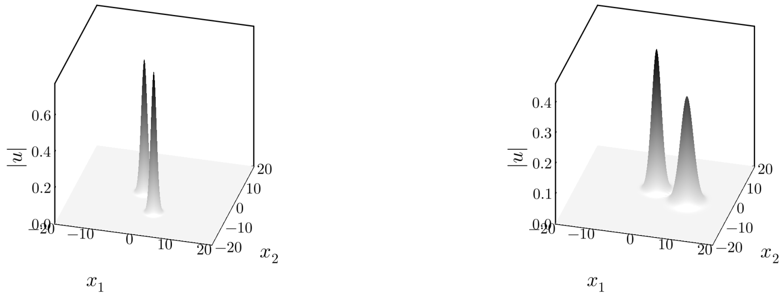
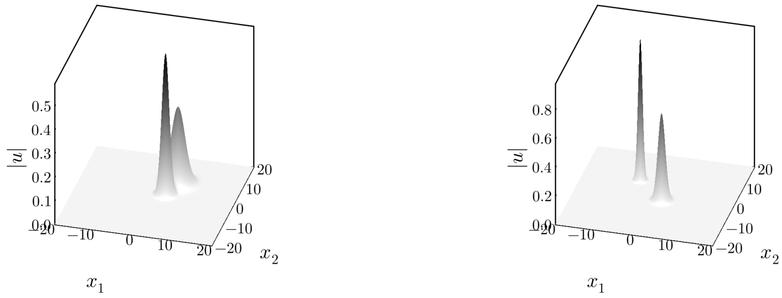


(a) $t = 0$ (b) $t = 0.6$



(c) $t = 1.2$ (d) $t = 1.8$



(e) $t = 2.4$ (f) $t = 3.0$

Fig. 3.: Absolute value of the approximate solution to the weakly-interacting rotating soliton example.

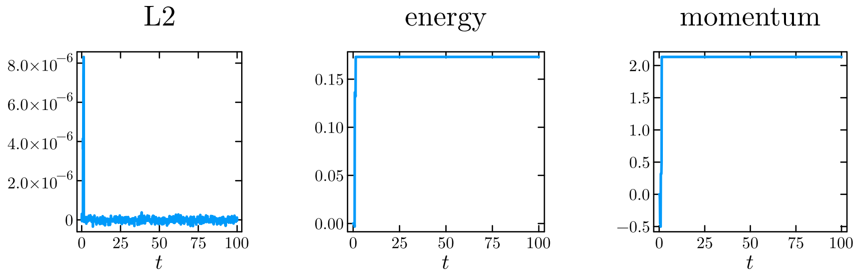


Fig. 4.: Time evolution of the relative conservative quantities: L^2 norm (left), energy (center) and momentum (right), for the two modulated solitons with strong interactions. Nonlinearity parameter $\mu = 1$.

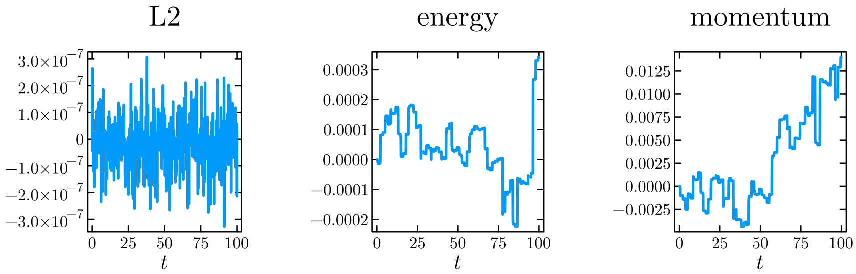


Fig. 5.: Time evolution of the relative conservative quantities: L^2 norm (left), energy (center) and momentum (right), for the two modulated solitons with strong interactions. Nonlinearity parameter $\mu = 10^{-3}$.