Modulation algorithm for the nonlinear Schrödinger equation

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Abstract

Based on recent ideas, stemming from the use of *bubbles*, we discuss an algorithm for the numerical simulation of the cubic nonlinear Schrödinger equation with harmonic potential in any dimension, which could be easily extended to other polynomial nonlinearities. For the linear part of the equation, the algorithm consists in discretizing the initial function as a sum of modulated complex functions, each one having its own set of parameters, and then updating the parameters exactly so that the modulated function remains a solution to the equation. When cubic interactions are introduced, the Dirac-Frenkel-MacLachlan principle is used to approximate the time evolution of parameters. We then obtain a grid-free algorithm in any dimension, and it is compared to a spectral method on numerical examples.

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1 Introduction

We are interested in approximating numerically the solution $\psi(t, x)$ to the cubic nonlinear Schrödinger equation with harmonic potential,

$$i\partial_t\psi + \Delta_x\psi - |x|^2\psi = \psi|\psi|^2, \quad x \in \mathbb{R}^d, \tag{cNLS}$$

where $d \geq 1$, $|\cdot|$ denotes the usual Euclidian norm over $\mathbb{R}^d$, and Δ_x denotes the Laplace operator over $\mathbb{R}^d$: $\Delta_x = \sum_{i=1}^{d} \partial^2_{x_i}$. This equation is also sometimes called *time-dependent Gross-Pitaevskii equation* [CCP+00, BJM03, Wan17, TTK22]. We focus on a cubic nonlinearity for the sake of clarity, but we emphasize the fact that everything we present is also applicable to other types of polynomial nonlinearities, *mutatis mudandis*. Similarly, the extension to the equation (1.4) – which is (cNLS) without the harmonic potential – is also straightforward.

Very recent works [MR18, FR20] suggest to discretize the solution ψ of (cNLS) as a sum of N modulated functions, which write as:

$$\psi(t, x) \approx u(t, x) := \sum_{j=1}^{N} u_j(t, x), \tag{1.1}$$

where

$$u_j(t,x) := \frac{A_j}{L_j} e^{i\gamma_j + iL_j\beta_j\cdot y_j - i\frac{B_j}{4}|y_j|^2} v_j(s_j,y_j), \quad \text{with} \quad \left| \begin{aligned} &\frac{\mathrm{d}s_j}{\mathrm{d}t} := \frac{1}{L_j^2}, \\ &y_j := \frac{x-X_j}{L_j}, \end{aligned} \right. \tag{1.2}$$

and $N \in \mathbb{N}^*$. In the cited works, the modulated functions u_j are called *bubbles*. Throughout this work, we may refer to the variables (s_j, y_j) as the *modulation frame* of the bubble labelled j.

The time dependence of the parameters $A_j, L_j, B_j, X_j, \beta_j, \gamma_j$ has not been written in (1.2) 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 (1.1) into (cNLS) in order to obtain ODEs for the parameters.

The idea of relying on time-dependent parameters to represent the solution, or an approximation, is not new and has been widely studied in the linear case, *i.e.* when the cubic nonlinearity is replaced by some multiplication with a potential. When the v_j are chosen as Gaussian functions, it has been called *Variational Gaussian wave packets* and extensively analyzed by Lasser and Lubich [LL20], where they applied the Dirac-Frenkel-MacLachlan principe (DFMP) to the linear Schrödinger equation with potential.

More generally, this type of method using Gaussian functions is widely used in the field of Chemical Physics [Hel76, HH87, CK90, WRB04, AKLP22]. The different methods used are variations of the same idea, and possess many names: superposition of Gaussian Wavepackets, Gaussian beams, Thawed Gaussians, Frozen Gaussian... All of these algorithms simply consist in applying a Dirac-Frenkel-MacLachlan principle to linear Schrödinger equations, the difference lying in how the parameters are updated. For example, the Thawed Gaussian method allows the width matrix to be time-dependent while the Frozen Gaussian does not.

Let us now explain the main ideas underlying the full modulation (1.2) – developed in various works, see for instance [MR18, FR20] and the references therein – and why it is particularly adapted to the nonlinear case.

Consider for instance the case of one bubble, *i.e.* $N = 1$. When plugging the ansatz (1.2) into (cNLS), we obtain an equation of the form

$$i\partial_s v + \Delta_y v - |y|^2 v - |v|^2 v + P(s; y, \partial_y)v = 0,$$

where $P(s; y, \partial_y)$ is a quadratic operator in y and ∂_y, which depends on time s through the parameters $(A, L, B, X, \beta, \gamma)$ and their time derivatives with respect to s. See (2.5) for more precise detail. It is then possible to choose the parameters in such a way that for instance $P(s; y, \partial_y)v = -\lambda v$ for some $\lambda \in \mathbb{R}$, and to take v as a soliton solution of the stationary equation

$$-\Delta_y v + |y|^2 v + |v|^2 v = \lambda v. \tag{1.3}$$

This yields a differential system to be solved by the parameters $(A, L, B, X, \beta, \gamma)$ which is given below by (2.10). It turns out that these equations form a *completely integrable Poisson system* that can be solved, and the solution for a single bubble can be thus taken as a *modulated soliton*.

In other words, taking $v_j = v$ when $N = 1$, a solution of the nonlinear equation (1.3) yields an exact solution $u_j = u$ under the form (1.2) of (cNLS).

This kind of approach has been used successfully in various situations from a theoretical point of view, see [MR05, MR18, FR20, MRRS20] and the references therein. Typically, when $N \geq 2$, several modulated solitons interact and this can produce finite time blow-up of growth of Sobolev norm phenomena. A large part of the analysis relies on the ability of calculating nonlinear interactions between two modulated solitons. This can be done for instance in an integrable situation, e.g. the Szegö equation [GLPR18].

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

$$i\partial_s \psi + \Delta_x \psi = \psi |\psi|^2, \quad x \in \mathbb{R}^d \tag{1.4}$$

on an unbounded time interval. In this case, the modulation equations generate the so-called *lens* transform, see for instance [Car21]. Note that our algorithms could be 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 [Ber20], where the time coefficients can be seen as specific time changes s in the modulation equations.

Inspired by these successful theoretical works, we retain the idea of approximating solutions to (cNLS) by modulating the parameters A_j, L_j, B_j, X_j, β_j, γ_j in such a way that $v_j(s_j, x)$ satisfies a *smoother in time* equation – typically a stationary soliton equation. However, from the numerical point of view, choosing the v_j as stationary solitons would require first to solve explicitly the nonlinear equation (1.3) and more problematically, to estimate numerically the nonlinear interactions between the modulated solitons by using the Dirac-Frenkel-MacLachlan principle. The latter consists essentially in a projection onto the manifold of modulated solitons, which is in practice very difficult to evaluate numerically. Moreover, one is naturally interested in using a splitting strategy between the linear and nonlinear parts, which would typically destroy the soliton structure in the equation. Following this idea, we split the Schrödinger equation (cNLS) into the linear part

$$i\partial_t \psi + \Delta_x \psi - |x|^2 \psi = 0, \tag{HO}$$

and the nonlinear part

$$i\partial_t \psi = \psi |\psi|^2. \tag{cNLS-nonLin.}$$

The linear equation (HO) is also called the Harmonic Oscillator. Traditional well-known numerical schemes are based on this abstract decomposition and it is easy to determine high-order splitting methods obtained by solving alternately the linear and nonlinear parts, like Lie, Strang Splitting or triple jump composition, see for instance [MQ02, HLW06, CCFM17]. However, the approximation of the solution to each of these two parts remains to be done using time and space discretizations. They are traditionally solved using grid-based numerical schemes (see for instance [BJM03, QY10, Fao12, Wan17, Ber20]). The computational complexity of grid-based methods is always an issue due to the bad scaling with respect to the dimension. Fortunately, using the modulation techniques given above, the solution to the linear part (HO) can be simulated exactly, in a straightforward manner, and very efficiently by considering Hermite decomposition of the functions v_j. The computational cost for the simulation of the linear part only is $\mathcal{O}(N \cdot d)$ – recall N is the number of bubbles and d the dimension – to be compared with grid-based complexities of order $\mathcal{O}(M^d)$ where M would be the number of discretization points in each dimension.

To approximate the solution to the nonlinear part (cNLS-nonLin.), we use the Dirac-Frenkel-MacLachlan principle. In theory, when the v_j are finite sums of Hermite polynomials, the calculation of the interactions boils down to the computation of integrals of products of Hermite functions in different modulation frames, which *a priori* can be done in a systematic way. In practice, these computations can get heavy and to simplify them we will give the explicit result of the Gaussian case in this paper.

In the end, we thus obtain an algorithm for modulated Gauss-Hermite functions, which can be easily implemented numerically, is grid-free, and is also able to capture high oscillations of the solution.

The paper is organized as follows. Section 2 is devoted to (HO) for a general bubble decomposition. We recall some conservation laws obtained when considering *bubbles* in (cNLS), and exhibit *universal modulation equations* which have a completely integrable Hamiltonian structure (see for instance [LR05, HLW06] for more details about completely integrable Hamiltonian structures). Analytical formula for all of the modulation parameters can then be made explicit by decomposing the v_j into the Hermite basis.

We focus in Section 3 on (cNLS-nonLin.), which takes into account cubic interactions. The nonlinearity that is introduced is the core of difficulties arising in the Schrödinger equation, and it is hopeless to look for exact solutions in the general case. The proposed approach uses the Dirac-Frenkel-MacLachlan principle to obtain modulation equations in the case of Gaussian functions v_j. The choice of Gaussian functions allows to perform most computations exactly, and to avoid numerical quadratures or delicate calculations of integrals of multiple products of Hermite functions. This allows us to take into account as many bubbles as one desires at the cost of a computational complexity of order $\mathcal{O}(N^4 d + d^3 N^3)$. Here, N is the total number of bubbles and d the dimension. The fourth power of N is due to polynomial interactions of order three. This algorithm almost does not suffer from the well-known "curse of dimensionality" since it is at most polynomial with respect to the dimension d.

Finally, Section 4 is dedicated to illustrating numerically the fine details that are obtainable with the Dirac-Frenkel-MacLachlan principle, as well as the long-time behavior, compared to a FFT-based spectral scheme. Our experiments show that, if the initial data is discretized "nicely", the given algorithm yields satisfying results.

2 The Harmonic Oscillator

In this section we focus onto the linear part of the cubic Non Linear Schrödinger equation, namely the Harmonic Oscillator (HO).

2.1 Conservation Laws

We recall classical laws for the Harmonic oscillator equation (see for instance [Tao06, KV13]). Let ψ be the solution to (HO).

Lemma 2.1 (Conserved quantities in dimension $d = 2$)**.** *We consider a two-parameter family of equations containing* (HO) *and* (cNLS)*:*

$$i\partial_t \psi + \mu(\Delta\psi - |x|^2\psi) = \lambda|\psi|^2\psi, \quad \mu, \lambda \in \mathbb{R}.$$

The (radial) conservation laws are mass $\|\psi\|_{\mathbb{L}^2}$*, energy*

$$E_{\mu,\lambda} = \frac{\mu}{2}\langle H\psi, \psi\rangle + \frac{\lambda}{4}\left\langle |\psi|^2\psi, \psi\right\rangle,$$

where $H = -\Delta + |x|^2$ *and* $\langle f, g\rangle := \int_{\mathbb{R}^d} f\bar{g}$*, and momentum*

$$M_{\mu,\lambda} = \left(E_{\mu,\lambda} - \mu\|x\psi\|^2_{\mathbb{L}^2}\right)^2 + \mu^2\left(\Im\int x\cdot\nabla\psi\bar{\psi}\right)^2,$$

and the same applied to any power $(-H)^s\psi$*. There also holds the non radial conservation law*

$$\mathcal{P}_j = \frac{1}{4}\left(\Im\int \partial_j\psi\bar{\psi}\right)^2 + \mu^2\left(\int x_j|\psi|^2\right)^2, \quad j = 1, 2.$$

Proof. See Appendix A. □

2.2 Renormalized flow

By linearity of the Harmonic oscillator part, we can reduce the problem to calculating the evolution of the decomposition (1.2) for only one bubble v_j. Recall the expression of $u(t, x)$:

$$u(t,x) = \frac{A}{L}e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2}v(s,y), \quad y = \frac{x - X(t)}{L(t)}, \ \frac{\mathrm{d}s}{\mathrm{d}t} = \frac{1}{L(t)^2}. \tag{2.1}$$

We compute, in dimension $d \geq 1$:

$$\Delta_x u = \frac{Ae^{i\gamma}}{L^3}\Delta_y\left[e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}v(s,y)\right],$$

and

$$\partial_k\left[e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}v\right] = e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}\left[\partial_k v + i\left(L\beta_k - \frac{B}{2}y_k\right)v\right], \quad k = 1, \dots, d, \tag{2.2}$$

and

$$\begin{aligned}\partial_k^2\left[e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}v\right] &= e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}\\ &\times\left[\partial_k^2 v + i\left(L\beta_k - \frac{B}{2}y_k\right)\partial_k v - i\frac{B}{2}v + i\left(L\beta_k - \frac{B}{2}y_k\right)\left[\partial_k v + i\left(L\beta_k - \frac{B}{2}y_k\right)v\right]\right]\\ &= e^{iL\beta\cdot y - i\frac{B}{4}|y|^2}\left[\partial_k^2 v + i\left(2L\beta_k - By_k\right)\partial_k v + \left(-i\frac{B}{2} - L^2\beta_k^2 + LB\beta_k y_k - \frac{B^2}{4}y_k^2\right)v\right].\end{aligned}$$

Hence,

$$\begin{aligned}\Delta_x u = \frac{A}{L^3}&e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2}v\\ &\times\left[\Delta_y v + i\left(2L\beta - By\right)\cdot\nabla v + \left(-i\frac{B}{2}d - L^2|\beta|^2 + LB\beta\cdot y - \frac{B^2}{4}|y|^2\right)v\right].\end{aligned}$$

We have

$$-|x|^2 u = -\frac{A}{L}e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2}\left|Ly + X\right|^2 v$$

$$= \frac{A}{L^3} e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2} \left(-L^4|y|^2 - 2L^3 X\cdot y - L^2|X|^2\right) v,$$

thus

$$\begin{aligned}(\Delta_x - |x|^2)u = \frac{A}{L^3} e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2} \Big\{ &\Delta_y v - iB\left(\frac{d}{2}v + \Lambda v\right) - L^2\left(|\beta|^2 + |X|^2\right) v \\ &+ 2iL\beta\cdot\nabla v + \left(LB\beta - 2L^3 X\right)\cdot yv + \left(-\frac{B^2}{4} - L^4\right)|y|^2 v\Big\},\end{aligned} \tag{2.3}$$

where we denoted $\Lambda v := y\cdot\nabla v$. We now compute

$$\begin{aligned}\partial_t u &= \partial_t\left(e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L}v(s,y)\right)\\ &= e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L}\left[\partial_t v + \frac{A_t}{A}v - \frac{L_t}{L}(v + \Lambda v) - \frac{X_t}{L}\cdot\nabla v\right]\\ &\quad + e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L} iv\\ &\qquad\times\Big[\gamma_t + \beta_t\cdot(x-X) - \beta\cdot X_t - \frac{B_t}{4L^2}|x-X|^2\\ &\qquad\qquad + \frac{2L_t B}{4L^3}|x - X(t)|^2 + \frac{2B}{4L^2}(x-X)\cdot X_t\Big]\\ &= e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L^3}\left[\partial_s v + \frac{A_s}{A}v - \frac{L_s}{L}(v+\Lambda v) - \frac{X_s}{L}\cdot\nabla v\right]\\ &\quad + e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L^3} iv\\ &\qquad\times\left[\gamma_s + L\beta_s\cdot y - \beta\cdot X_s - \frac{B_s}{4}|y|^2 + \frac{2L_s B}{4L}|y|^2 + \frac{B}{2}y\cdot\frac{X_s}{L}\right],\end{aligned}$$

and hence

$$\begin{aligned}i\partial_t u = e^{i\gamma + i\beta\cdot(x-X) - i\frac{B}{4L^2}|x-X|^2}\frac{A}{L^3}\Big\{ &i\partial_s v + (-\gamma_s + \beta\cdot X_s)v + \left(\frac{A_s}{A} - \frac{L_s}{L}\right)iv - \frac{L_s}{L}i\Lambda v\\ &- i\frac{X_s}{L}\cdot\nabla v + \left(-L\beta_s - \frac{BX_s}{2L}\right)\cdot yv + \left(\frac{B_s}{4} - \frac{B}{2}\frac{L_s}{L}\right)|y|^2 v\Big\}.\end{aligned} \tag{2.4}$$

This yields

$$\begin{aligned}i\partial_t u + \Delta_x u - |x|^2 u = \frac{A}{L^3} e^{i\gamma + iL\beta\cdot y - i\frac{B}{4}|y|^2}\Big\{ &i\partial_s v + \left(-\gamma_s + \beta\cdot X_s - L^2\left(|\beta|^2 + |X|^2\right)\right)v\\ &+ \left(\frac{A_s}{A} - \frac{L_s}{L} - B\frac{d}{2}\right)iv + \left(-\frac{L_s}{L} - B\right)i\Lambda v + i\left(2L\beta - \frac{X_s}{L}\right)\cdot\nabla v\\ &+ \left(-2L^3 X + LB\beta - L\beta_s - \frac{B}{2}\frac{X_s}{L}\right)\cdot yv\\ &+ \Delta_y v + \left[\frac{B_s}{4} - \left(\frac{B^2}{4} + L^4\right) - \frac{B}{2}\frac{L_s}{L}\right]|y|^2 v\Big\}(s,y).\end{aligned} \tag{2.5}$$

Once we have Equation (2.5), we are free to choose the parameters as we wish. A natural choice is to conjugate the equation back to the original one in variables (s,y), *i.e.*

to take

$$\left|\begin{array}{l}\gamma_s - \beta \cdot X_s + L^2\left(|\beta|^2 + |X|^2\right) = 0 \\ \dfrac{A_s}{A} - \dfrac{L_s}{L} - \dfrac{B}{2}d = 0 \\ -\dfrac{L_s}{L} - B = 0 \\ 2L\beta - \dfrac{X_s}{L} = 0 \\ -2L^3X + LB\beta - L\beta_s - \dfrac{BX_s}{2L} = 0 \\ \dfrac{B_s}{4} - \left(\dfrac{B^2}{4} + L^4\right) - \dfrac{B}{2}\dfrac{L_s}{L} = -1.\end{array}\right. \tag{2.6}$$

Certain choices may be more convenient than others, and (2.6) is chosen so that v only has to solve the stationary Harmonic Oscillator in the variables (s, y):

$$(i\partial_t + \Delta_x - |x|^2)u(t,x) = 0 \qquad \Longleftrightarrow \qquad (i\partial_s + \Delta_y - |y|^2)v(s,y) = 0. \tag{2.7}$$

Now we see that if v is decomposed in the Hermite basis, we can solve explicitly the previous equation in variable (s, y) and obtain the solution $u(t, x)$ after solving the differential system (2.6).

Any function statisfying equation (2.7) can be decomposed in the Hermite basis

$$\left\{\varphi_n := H_{n_1} \cdots H_{n_d} : n \in \mathbb{N}^d\right\},$$

where the function $H_k(z)$ denotes the Hermite function of order $k \in \mathbb{N}$, which satisfies the following diffferential equation:

$$H_k''(z) + (2k + 1 - z^2)H_k(z) = 0.$$

A straightforward calculation shows that

$$(-\Delta_y + |y|^2)\varphi_n = (2|n| + d)\varphi_n$$

where $|n| := \sum_{k=1}^d n_k$. Hence from a decomposition

$$v(0,y) = \sum_{n\in\mathbb{N}^d} v_n\varphi_n(y) \tag{2.8}$$

with $v_n \in \mathbb{C}$, we calculate that

$$v(s,y) = \sum_{n\in\mathbb{N}^d} v_n e^{-(2|n|+d)is}\varphi_n(y) \tag{2.9}$$

is solution of (2.7). It remains to obtain $u(t, x)$ solution of (HO). In order to do this, one simply needs to integrate (2.6) (which is independent of n in the Hermite decomposition), and to plug (2.9) into (2.1). In particular, we need to calculate the time $s(t)$ as a function of the original time t.

2.3 Integrability of the modulation equations

We rewrite (2.6) as

$$\left| \begin{aligned} &A_s = \frac{AB}{2}(d-2) \\ &L_s = -BL \\ &B_s = -4 + 4L^4 - B^2 \\ &X_s = 2L^2\beta \\ &\beta_s = -2L^2 X \\ &\gamma_s = L^2\left(|\beta|^2 - |X|^2\right). \end{aligned} \right. \tag{2.10}$$

In time t, as $\frac{\mathrm{d}}{\mathrm{d}s} = L^2 \frac{\mathrm{d}}{\mathrm{d}t}$, this system is

$$\left| \begin{aligned} &A_t = \frac{AB}{2L^2}(d-2) \\ &L_t = -\frac{B}{L} = -2L\partial_B \mathcal{E} \\ &B_t = -\frac{4}{L^2} + 4L^2 - \frac{B^2}{L^2} = 2L\partial_L \mathcal{E} \\ &X_t = 2\beta = \nabla_\beta \mathcal{R} \\ &\beta_t = -2X = -\nabla_X \mathcal{R} \\ &\gamma_t = |\beta|^2 - |X|^2, \end{aligned} \right. \tag{2.11}$$

with

$$\mathcal{E}(B,L) = \frac{1}{L^2}\left(1 + \frac{B^2}{4}\right) + L^2, \quad \text{and} \quad \mathcal{R}(X,\beta) = |X|^2 + |\beta|^2.$$

Let us write explicitly the Darboux-Lie transformation associated with the previous Poisson system, to obtain canonical Hamiltonian coordinates. We set

$$k = \frac{1}{2}\log L, \quad L = e^{2k},$$

and the system becomes

$$\left| \begin{aligned} &k_t = -\partial_B \mathcal{H} \\ &B_t = \partial_k \mathcal{H} \\ &X_t = \nabla_\beta \mathcal{H} \\ &\beta_t = -\nabla_X \mathcal{H} \\ &A_t = \frac{AB}{2}(d-2)e^{-4k} \\ &\gamma_t = |\beta|^2 - |X|^2, \end{aligned} \right. \tag{2.12}$$

with

$$\mathcal{H}(k,B,X,\beta) = \mathcal{E}(k,B) + \mathcal{R}(X,\beta) = e^{-4k}\left(\frac{B^2}{4} + 1\right) + e^{4k} + |X|^2 + |\beta|^2.$$

Lemma 2.2. *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*

$$E(h, a, \xi, \theta) = 4h + 2|a|^2, \tag{2.13}$$

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

$$\begin{aligned} a(t) &= a(0), \\ \theta(t) &= \theta(0) + 2t, \\ h(t) &= h(0), \\ \xi(t) &= \xi(0) - 4t. \end{aligned} \tag{2.14}$$

We have the explicit formulae:

$$\begin{aligned} A(t) &= A(0) \left(\frac{L(t)}{L(0)} \right)^{\frac{2-d}{2}}, \\ e^{4k(t)} &= L(t)^2 = 2h(t) - \cos(\xi(t)) \sqrt{4h(t)^2 - 1}, \\ B(t) &= 2 \sin(\xi(t)) \sqrt{4h(t)^2 - 1}, \\ X_i(t) &= \sin(\theta_i(t)) \sqrt{2a_i(t)}, \quad i = 1, \dots, d, \\ \beta_i(t) &= \cos(\theta_i(t)) \sqrt{2a_i(t)}, \quad i = 1, \dots, d, \\ \gamma(t) &= \gamma(0) + \sum_{l=1}^{d} \frac{a_l(0)}{2} \left[\sin(2\theta_l(t)) - \sin(2\theta_l(0)) \right] \\ s(t) &= -\frac{1}{2} \arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan\left(\frac{\xi(0)}{2} - 2t \right) \right) \\ &\quad + \frac{1}{2} \arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan\left(\frac{\xi(0)}{2} \right) \right) + m_t \frac{\pi}{2}, \end{aligned} \tag{2.15}$$

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* $\frac{\xi(t)}{2} \in (m_0 - m_t)\pi + \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$.

The proof of this Lemma is given in Appendix B. If one knows the parameters $(A, L, B, X, \beta, \gamma)$, it suffices to apply (2.15) in order to update them. Then we combine these expressions with the decomposition (2.9) and the expression of $s(t)$ to obtain the expression of $u(t, x)$.

In practice, one knows the bubble's parameters and needs first to obtain action-angle variables. We have the following result:

Lemma 2.3. *The change of variables* $(L, B, X, \beta) \mapsto (h, a, \xi, \theta)$ *is explicit, and at time*

$t = 0$ we have

$$\begin{aligned} a_i(0) &= \frac{1}{2}\left(X_i(0)^2 + \beta_i(0)^2\right), i = 1, \dots, d, \\ \theta_i(0) &= \arctan\left(\frac{X_i(0)}{\beta_i(0)}\right), i = 1, \dots, d, \\ h(0) &= \frac{L(0)^4 + 1 + \frac{B(0)^2}{4}}{4L(0)^2}, \\ \xi(0) &= \arctan\left(\frac{B(0)}{4h(0) - 2L(0)^2}\right), \end{aligned} \tag{2.16}$$

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 (2.16) 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 $t \mapsto s(t)$.

The proof of Lemma 2.3 is given in Appendix C. Note that to define $\xi(0)$ we could also use equation (B.3), but this is not appropriate from a computational point of view. Some more details are given in Remark 2.1.

Using Lemmata 2.2 and 2.3, we are now able to obtain a straightforward numerical algorithm which simulates exactly the evolution of bubbles according to the Harmonic Oscillator on a time interval $[0, T]$. It is described in Algorithm 1.

Algorithm 1 Solving the Harmonic oscillator with Bubbles

```
for j = 1, ..., N do                                  ▷ j denotes a bubble's index in (1.1)
    Use (2.16) to get the action-angle variables (h, a, ξ, θ) at time 0.
    Use (2.14) to update the variables (h, a, ξ, θ) up to time T.
    Use (2.15) to get the parameters of bubble u_j at time T.
    Use (2.9) to update the Hermite decomposition of the bubble.
end for
```

Remark 2.1 (Numerical considerations). Here are a few remarks about Algorithm 1:

- When applying equation (2.16) to obtain the action-angle variables from the bubbles' parameters, it is advised to use the function $\arctan2(y, x)$ instead of $\arctan(y/x)$ because it allows to obtain an angle lying in $(-\pi, \pi]$ instead of $(-\pi/2, \pi/2]$ by taking into account the signs of both x and y. This is also the reason why we do not define $\xi(0)$ by (B.3). Moreover most numerical implementations of arctan2 return a finite value for $\arctan2(0, 0)$, which avoids the manual tuning of a numerical threshold to know whether $a_i(0)$ or $h(0)$ vanish numerically or not. We recall that in this case the exact value returned does not impact the behavior of $t \mapsto (L(t), B(t), X(t), \beta(t), \gamma(t), s(t))$.
- The family $\left\{\varphi_n = H_{n_1} \cdots H_{n_d} : n = (n_1, \dots, n_d) \in \mathbb{N}^d\right\}$ is an orthonormal family of $\mathbb{L}^2(\mathbb{R}^d)$, hence the discretization of any initial condition is done by calculating (or choosing) the Hermite coefficients of the functions v_j in the decomposition (1.1).

- The algorithm yields an exact solution as soon as the initial data is a sum of bubbles. If not, then the only error committed is the discretization error when approximating the initial condition $\psi(t=0)$ by the ansatz (1.1).
- This numerical algorithm does not need any discretization in time nor in space.
- The solution obtained is the *exact* solution of the equation (HO) defined on the whole space $\mathbb{R}^d$, and no numerical boundary conditions are needed.

3 The Dirac-Frenkel-MacLachlan principle

In this section we consider the Schrödinger equation (cNLS). As it has been explained before, the equation consists in two parts: the linear part (HO), and the nonlinear part (cNLS-nonLin.). Section 2 was dedicated to solving the Harmonic oscillator, namely the linear part. We are interested now in solving the nonlinear part, and as it is usually done for numerical simulations, we will use a splitting method (see for instance [MQ02, HLW06, CCFM17]). This will allow us to solve (cNLS) by solving separately (HO) and (cNLS-nonLin.), one after the other. By doing so, a splitting error is made, which depends on the timestep Δt, and the order of the error depends on the specific splitting method. It is also possible to apply high-order splitting methods.

We focus on approximating numerically the solution to (cNLS-nonLin.):

$$i\partial_t\psi = \psi|\psi|^2.$$

We are free to use any method we want, but one has to keep in mind that Algorithm 1 solves (HO) exactly when ψ is expressed under the form (1.1), i.e. as a sum of bubbles. Therefore we would like the approximate solution to (cNLS-nonLin.) to keep this particular form. This naturally calls for the use of the Dirac-Frenkel-MacLachlan principle (abbreviated DFMP). For more details, see [LL20, Sect. 3].

In theory, the calculation can be performed in a very general situation, when all the v_j involved in (1.1)-(1.2) are given in terms of Hermite polynomials. In essence, the only difficulty lies in the evaluation of general integrals of products of Hermite functions in different modulation frames, which can be done using generating functions techniques for instance. Another alternative would be to use nonlinear solitons and rely on numerical evaluations of the corresponding integrals.

In the remainder of this paper, we will consider the primary case by considering $\mathcal{M}$ be a manifold of complex-valued Gaussian functions:

$$\mathcal{M} := \left\{ u \in \mathbb{L}^2(\mathbb{R}^d) \,\middle|\, \begin{array}{c} u(x) = \sum_{j=1}^{N} \frac{A_j}{L_j} e^{i\gamma_j + i\beta_j\cdot(x-X_j) - \frac{2+iB_j}{4L_j^2}|x-X_j|^2}, \\ A_j, B_j, \gamma_j \in \mathbb{R},\ L_j \in \mathbb{R}_+^*,\ X_j, \beta_j \in \mathbb{R}^d \end{array} \right\}. \tag{3.1}$$

Remark 3.1. Note that the functions $e^{-\frac{|y|^2}{2}}$ are simply $\varphi_{(0,\ldots,0)}(y) = H_0(y_1)\cdots H_0(y_d)$, hence we can use Section 2.3 for the linear part.

We look for a function $u \in \mathcal{M}$ that solves (cNLS-nonLin.) on $\mathcal{M}$. More precisely, u is defined such that its time derivative lies in the tangent space of $\mathcal{M}$ at u, $\mathcal{T}_{u(t)}\mathcal{M}$, and such that the residual of equation (cNLS-nonLin.) is orthogonal to the tangent space. That is,

$$\begin{aligned} &\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \text{such that} \\ &\langle f, i\partial_t u(t) - u(t)|u(t)|^2\rangle = 0, \, \forall f \in \mathcal{T}_{u(t)}\mathcal{M}. \end{aligned} \tag{3.2}$$

Remark 3.2. The definition of $\partial_t u(t)$ via (3.2), initially proposed by Dirac and Frenkel [Dir30, Fre34], has been later criticized by MacLachlan [McL64]. He proposed an alternative approach, which would consist in minimizing the quantity

$$\left|\left|i\partial_t u(t) - |u(t)|^2 u(t)\right|\right|^2.$$

However, the two formulations are equivalent if the tangent space $\mathcal{T}_{u(t)}\mathcal{M}$ is $\mathbb{C}$-linear [BLKVL88]. This is the case here because multiplying by the complex unit i simply amounts to $\gamma_j \mapsto \gamma_j + \frac{\pi}{2}$. Therefore, the approaches by Dirac-Frenkel and MacLachlan are equivalent.

Let $B_{u(t)}$ be a basis of $\mathcal{T}_{u(t)}\mathcal{M}$, then (3.2) is equivalent to

$$\begin{aligned} &\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \text{such that} \\ &\langle f, i\partial_t u(t)\rangle = \langle f, u(t)|u(t)|^2\rangle, \, \forall f \in B_{u(t)}. \end{aligned} \tag{3.3}$$

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

$$\begin{aligned} B_{u(t)} &= \left\{ e^{i\Gamma_j(y_j) - \frac{|y|^2}{2}}, (y_j)_1 e^{i\Gamma_j(y_j) - \frac{|y_j|^2}{2}}, \ldots, (y_j)_d e^{i\Gamma_j(y_j) - \frac{|y_j|^2}{2}}, |y_j|^2 e^{i\Gamma_j(y_j) - \frac{|y_j|^2}{2}} : j = 1, \ldots, N \right\}, \\ &=: \{b_{j,1}, b_{j,2}, \ldots, b_{j,d+1}, b_{j,d+2} : j = 1, \ldots, N\}, \end{aligned} \tag{3.4}$$

where we defined

$$\Gamma_j(y_j) := \gamma_j + L_j\beta_j \cdot y_j - \frac{B_j}{4}|y_j|^2.$$

Thus, (3.3) is equivalent to

$$\langle i\partial_t u(t), b_{j,l}\rangle = \langle u|u|^2, b_{j,l}\rangle, \quad j = 1, \ldots, N, \quad l = 1, \ldots, d+2. \tag{3.5}$$

The next step consists in expressing (3.5) as a linear system involving the parameters of the bubbles and their time derivative. We then solve the linear system, which yields ODEs on the parameters that we can integrate numerically. The main advantage of this approach is that it guarantees to keep the approximate solution of (cNLS-nonLin.) as a sum of N bubbles.

In order to obtain the linear system, we first have to get the expression of $i\partial_t u(t)$ when $v(y) = e^{-\frac{|y|^2}{2}}$: by summing (2.4) over $j = 1, \ldots, N$, one has

$$\begin{aligned} i\partial_t u = \sum_{j=1}^{N} \frac{u_j}{L_j^2} \Bigg\{ &|y_j|^2 \left(i\frac{(L_j)_s}{L_j} - \frac{B_j(L_j)_s}{2L_j} + \frac{(B_j)_s}{4} \right) \\ &+ y_j \cdot \left(-L_j(\beta_j)_s + i\frac{(X_j)_s}{L_j} - \frac{B_j}{2L_j}(X_j)_s \right) \\ &+ i\frac{(A_j)_s}{A_j} - i\frac{(L_j)_s}{L_j} + \beta \cdot (X_j)_s - (\gamma_j)_s \Bigg\}. \end{aligned} \tag{3.6}$$

More concisely, we have

$$
\begin{aligned}
i\partial_t u &= \sum_{j=1}^{N} \frac{A_j}{L_j^3} e^{i\Gamma_j - \frac{|y_j|^2}{2}} \Big\{ |y_j|^2 \left(E_j^{(5)} + iE_j^{(6)} \right) \\
&\qquad\qquad + y_j \cdot \left(E_j^{(3)(1,\ldots,d)} + iE_j^{(4)(1,\ldots,d)} \right) \\
&\qquad\qquad + \left(E_j^{(1)} + iE_j^{(2)} \right) \Big\} \\
&= \sum_{j=1}^{N} \frac{A_j}{L_j^3} \Big\{ b_{j,1} \left(E_j^{(1)} + iE_j^{(2)} \right) + b_{j,2} \left(E_j^{(3)(1)} + iE_j^{(4)(1)} \right) \\
&\qquad\qquad \cdots + b_{j,d+1} \left(E_j^{(3)(d)} + iE_j^{(4)(d)} \right) + b_{j,d+2} \left(E_j^{(5)} + iE_j^{(6)} \right) \Big\},
\end{aligned}
\tag{3.7}
$$

where

$$
\begin{aligned}
E_j^{(1)} &:= \beta_j \cdot (X_j)_s - (\gamma_j)_s, & E_j^{(2)} &:= \frac{(A_j)_s}{A_j} - \frac{(L_j)_s}{L_j}, \\
E_j^{(3)(l)} &:= -L_j((\beta_j)_l)_s - \frac{B_j}{2L_j}((X_j)_l)_s, & E_j^{(4)(l)} &:= \frac{((X_j)_l)_s}{L_j}, \qquad l = 1, \ldots, d, \\
E_j^{(5)} &:= \frac{(B_j)_s}{4} - \frac{B_j (L_j)_s}{2L_j}, & E_j^{(6)} &:= \frac{(L_j)_s}{L_j},
\end{aligned}
\tag{3.8}
$$

and where $E_j^{(k)(1,\ldots,d)}$ denotes the vector $(E_j^{(k)(1)}, \ldots, E_j^{(k)(d)})$. We recall the subscript $_s$ denotes the derivative with respect to time s.

According to (3.5), we then want to project $i\partial_t u(t)$ against every element of $B_{u(t)}$. We obtain the following linear system:

$$
\mathbf{AE} = S, \tag{3.9}
$$

where

$$
\mathbf{A} := \begin{pmatrix} \langle b_{1,1}, b_{1,1} \rangle & \langle b_{1,2}, b_{1,1} \rangle & \ldots & \langle b_{N,d+1}, b_{1,1} \rangle & \langle b_{N,d+2}, b_{1,1} \rangle \\ \vdots & & & & \vdots \\ \langle b_{1,1}, b_{N,d+2} \rangle & \langle b_{1,2}, b_{N,d+2} \rangle & \ldots & \langle b_{N,d+1}, b_{N,d+2} \rangle & \langle b_{N,d+2}, b_{N,d+2} \rangle \end{pmatrix} \in \mathbb{C}^{(d+2)N,(d+2)N},
$$

$$\mathbf{E} := \begin{pmatrix} \frac{A_1}{L_1^3}\left(E_1^{(1)} + iE_1^{(2)}\right) \\ \frac{A_1}{L_1^3}\left(E_1^{(3)(1)} + iE_1^{(4)(1)}\right) \\ \vdots \\ \frac{A_1}{L_1^3}\left(E_1^{(3)(d)} + iE_1^{(4)(d)}\right) \\ \frac{A_1}{L_1^3}\left(E_1^{(5)} + iE_1^{(6)}\right) \\ \vdots \\ \frac{A_j}{L_j^3}\left(E_j^{(1)} + iE_j^{(2)}\right) \\ \frac{A_j}{L_j^3}\left(E_j^{(3)(1)} + iE_j^{(4)(1)}\right) \\ \vdots \\ \frac{A_j}{L_j^3}\left(E_j^{(3)(d)} + iE_j^{(4)(d)}\right) \\ \frac{A_j}{L_j^3}\left(E_j^{(5)} + iE_j^{(6)}\right) \\ \vdots \\ \frac{A_N}{L_N^3}\left(E_N^{(1)} + iE_N^{(2)}\right) \\ \frac{A_N}{L_N^3}\left(E_N^{(3)(1)} + iE_N^{(4)(1)}\right) \\ \vdots \\ \frac{A_N}{L_N^3}\left(E_N^{(3)(d)} + iE_N^{(4)(d)}\right) \\ \frac{A_N}{L_N^3}\left(E_N^{(5)} + iE_N^{(6)}\right) \end{pmatrix} \in \mathbb{R}^{(d+2)N},$$

and

$$\mathbf{S} := \begin{pmatrix} \langle u|u|^2, b_{1,1}\rangle \\ \vdots \\ \langle u|u|^2, b_{N,d+2}\rangle \end{pmatrix} \in \mathbb{C}^{(d+2)N}.$$

The matrix $\mathbf{A}$ is the Gram matrix of the family $B_{u(t)}$, which obviously depends on time. In order to solve the linear system (3.9) we shall use the Moore-Penrose pseudo-inverse which always exists, and which corresponds to the Least Squares solution if the matrix $\mathbf{A}^*\mathbf{A}$ is invertible. The matrix $\mathbf{A}$ is invertible if and only if $B_{u(t)}$ is a linearly independent family of $\mathbb{L}^2(\mathbb{R}^d)$. We can already notice that if two bubbles have the same parameters then the family will be linearly dependent: this is why the Moore-Penrose pseudo-inverse is used instead of $\mathbf{A}^{-1}$, which is not always well-defined.

Once the linear system (3.9) is solved, we obtain $\mathbf{E}$, from which we can update the modulation parameters. In order to solve numerically the linear system, we shall rewrite it under a more convenient form. Let $\mathbf{A}_\Re := \Re(\mathbf{A})$, $\mathbf{A}_\Im := \Im(\mathbf{A})$, $\mathbf{E}_\Re := \Re(\mathbf{E})$, $\mathbf{E}_\Im := \Im(\mathbf{E})$, $\mathbf{S}_\Re := \Re(\mathbf{S})$, and $\mathbf{S}_\Im := \Im(\mathbf{S})$. Then, (3.9) writes:

$$\begin{aligned} \mathbf{A}\mathbf{E} = \mathbf{S} &\iff (\mathbf{A}_\Re + i\mathbf{A}_\Im)(\mathbf{E}_\Re + i\mathbf{E}_\Im) = \mathbf{S}_\Re + i\mathbf{S}_\Im \\ &\iff \begin{cases} \mathbf{A}_\Re\mathbf{E}_\Re - \mathbf{A}_\Im\mathbf{E}_\Im = \mathbf{S}_\Re \\ \mathbf{A}_\Im\mathbf{E}_\Re + \mathbf{A}_\Re\mathbf{E}_\Im = \mathbf{S}_\Im \end{cases} \\ &\iff \begin{pmatrix} \mathbf{A}_\Re & -\mathbf{A}_\Im \\ \mathbf{A}_\Im & \mathbf{A}_\Re \end{pmatrix} \begin{pmatrix} \mathbf{E}_\Re \\ \mathbf{E}_\Im \end{pmatrix} = \begin{pmatrix} \mathbf{S}_\Re \\ \mathbf{S}_\Im \end{pmatrix}. \end{aligned} \tag{3.10}$$

It is more convenient to solve (3.10) than (3.9), because we only have to deal with real matrices and vectors.

Remark 3.3. We first tried to solve (3.9) using the Moore-Penrose pseudo-inverse, however it yielded incomprehensible results. After some investigation, we found out that the issue seems to be the complex numbers involved, and that they do not mix well with the pseudo-inverse. The linear system (3.10) yields much better results.

Once (3.10) is solved, we have to update the bubbles parameters according to (3.8). The parameters of the bubble labelled j can be updated with $(\mathbf{E}_\Re)_k$ and $(\mathbf{E}_\Im)_k$ for $k = (d+2)(j-1)+1, \dots, (d+2)j$. For the sake of clarity, let $\mathbf{F} := \begin{pmatrix} \mathbf{E}_\Re \\ \mathbf{E}_\Im \end{pmatrix}$. Then

$$\frac{A_j}{L_j^3}\begin{pmatrix} E_j^{(1)} \\ E_j^{(3)(1)} \\ \vdots \\ E_j^{(3)(d)} \\ E_j^{(5)} \\ E_j^{(2)} \\ E_j^{(4)(1)} \\ \vdots \\ E_j^{(4)(d)} \\ E_j^{(6)} \end{pmatrix} = \begin{pmatrix} (\mathbf{E}_\Re)_{(d+2)(j-1)+1} \\ (\mathbf{E}_\Re)_{(d+2)(j-1)+2} \\ \vdots \\ (\mathbf{E}_\Re)_{(d+2)(j-1)+d+1} \\ (\mathbf{E}_\Re)_{(d+2)(j-1)+d+2} \\ (\mathbf{E}_\Im)_{(d+2)(j-1)+1} \\ (\mathbf{E}_\Im)_{(d+2)(j-1)+2} \\ \vdots \\ (\mathbf{E}_\Im)_{(d+2)(j-1)+d+1} \\ (\mathbf{E}_\Im)_{(d+2)(j-1)+d+2} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{(d+2)(j-1)+1} \\ \mathbf{F}_{(d+2)(j-1)+2} \\ \vdots \\ \mathbf{F}_{(d+2)(j-1)+d+1} \\ \mathbf{F}_{(d+2)(j-1)+d+2} \\ \mathbf{F}_{(d+2)N+(d+2)(j-1)+1} \\ \mathbf{F}_{(d+2)N+(d+2)(j-1)+2} \\ \vdots \\ \mathbf{F}_{(d+2)N+(d+2)(j-1)+d+1} \\ \mathbf{F}_{(d+2)N+(d+2)(j-1)+d+2} \end{pmatrix} =: \begin{pmatrix} F_j^{(1)} \\ F_j^{(3)(1)} \\ \vdots \\ F_j^{(3)(d)} \\ F_j^{(5)} \\ F_j^{(2)} \\ F_j^{(4)(1)} \\ \vdots \\ F_j^{(4)(d)} \\ F_j^{(6)} \end{pmatrix}$$

$$\iff \begin{pmatrix} \beta_j \cdot (X_j)_s - (\gamma_j)_s \\ -L_j(\beta_j)_s - \frac{B_j}{2L_j}(X_j)_s \\ \frac{(B_j)_s}{4} - \frac{B_j (L_j)_s}{2L_j} \\ \frac{(A_j)_s}{A_j} - \frac{(L_j)_s}{L_j} \\ \frac{(X_j)_s}{L_j} \\ \frac{(L_j)_s}{L_j} \end{pmatrix} = \frac{L_j^3}{A_j}\Re\begin{pmatrix} F_j^{(1)} \\ F_j^{(3)(1,\dots,d)} \\ F_j^{(5)} \\ F_j^{(2)} \\ F_j^{(4)(1,\dots,d)} \\ F_j^{(6)} \end{pmatrix}.$$

Hence

$$\begin{cases} \beta_j \cdot (X_j)_s - (\gamma_j)_s = F_j^{(1)}, \\ -L_j(\beta_j)_s - \dfrac{B_j}{2L_j}(X_j)_s = F_j^{(3)(1,\dots,d)}, \\ \dfrac{(B_j)_s}{4} - \dfrac{B_j(L_j)_s}{2L_j} = F_j^{(5)}, \\ \dfrac{(A_j)_s}{A_j} - \dfrac{(L_j)_s}{L_j} = F_j^{(2)}, \\ \dfrac{(X_j)_s}{L_j} = F_j^{(4)(1,\dots,d)}, \\ \dfrac{(L_j)_s}{L_j} = F_j^{(6)}, \end{cases} \iff \begin{cases} (A_j)_s = A_j\left(F_j^{(2)} + F_j^{(6)}\right), \\ (L_j)_s = L_j F_j^{(6)}, \\ (B_j)_s = 4F_j^{(5)} + 2B_j F_j^{(6)}, \\ (X_j)_s = L_j F_j^{(4)(1,\dots,d)}, \\ (\beta_j)_s = -\dfrac{1}{L_j}F_j^{(3)(1,\dots,d)} - \dfrac{B_j}{2L_j}F_j^{(4)(1,\dots,d)}, \\ (\gamma_j)_s = L_j\beta_j \cdot F_j^{(4)(1,\dots,d)} - F_j^{(1)}, \end{cases}$$

and with respect to time t,

$$\begin{cases} (A_j)_s = \dfrac{A_j}{L_j^2}\left(F_j^{(2)} + F_j^{(6)}\right), \\ (L_j)_s = \dfrac{1}{L_j}F_j^{(6)}, \\ (B_j)_s = \dfrac{4}{L_j^2}F_j^{(5)} + \dfrac{2}{L_j^2}B_jF_j^{(6)}, \\ (X_j)_s = \dfrac{1}{L_j}F_j^{(4)(1,\dots,d)}, \\ (\beta_j)_s = -\dfrac{1}{L_j^3}F_j^{(3)(1,\dots,d)} - \dfrac{B_j}{2L_j^3}F_j^{(4)(1,\dots,d)}, \\ (\gamma_j)_s = \dfrac{1}{L_j}\beta_j \cdot F_j^{(4)(1,\dots,d)} - \dfrac{1}{L_j^2}F_j^{(1)}, \end{cases} \tag{3.11}$$

3.1 Computing coefficients of the linear system (3.9)

In order to be able to compute $\mathbf{A}$ and $\mathbf{S}$, we give the exact expression of the inner products involved. For $j, l = 1, \dots, N$, let

$$\left| \begin{aligned} & z := \frac{2+iB_l}{4L_l^2} + \frac{2-iB_j}{4L_j^2}, \\ & a := \frac{X_l}{L_l^2} + \frac{X_j}{L_j^2}, \\ & \xi := \frac{B_j}{2L_j^2}X_j + \beta_j - \frac{B_l}{2L_l^2}X_l - \beta_l, \\ & C = \exp\left\{ i(\gamma_l - \gamma_j) - \frac{2+iB_l}{4L_l^2}|X_l|^2 - \frac{2-iB_j}{4L_j^2}|X_j|^2 - i\beta_l \cdot X_l + i\beta_j \cdot X_j \right\}. \end{aligned} \right. \tag{3.12}$$

Those quantities obviously depend on the indices j and l, but for clarity we do not write explicitly these dependences since they are pretty clear. Then, for $n, m = 1, \dots, d$,

$$\begin{aligned} \langle b_{l,1}, b_{j,1} \rangle &= C\widehat{f}(\xi) \\ \langle b_{l,n+1}, b_{j,1} \rangle &= \frac{C}{L_l}\left(\widehat{xf}_n - (X_l)_n\widehat{f}\right)(\xi) \\ \langle b_{l,d+2}, b_{j,1} \rangle &= \frac{C}{L_l^2}\left(\widehat{|x|^2 f} - 2X_l \cdot \widehat{xf} + |X_l|^2\widehat{f}\right)(\xi) \\ \langle b_{l,n+1}, b_{j,m+1} \rangle &= \frac{C}{L_jL_l}\left[\widehat{x_nx_mf} - (X_l)_n\widehat{x_mf} - (X_j)_m\widehat{x_nf} + (X_l)_n(X_j)_m\widehat{f}\right](\xi) \\ \langle b_{l,d+2}, b_{j,m+1} \rangle &= \frac{C}{L_l^2L_j}\Big[\widehat{x_m|x|^2f} - 2X_l \cdot \widehat{x_mxf} + |X_l|^2\widehat{x_mf} \\ &\qquad - (X_j)_m\widehat{|x|^2f} + 2(X_j)_mX_l \cdot \widehat{xf} - |X_l|^2(X_j)_m\widehat{f}\Big](\xi) \\ \langle b_{l,d+2}, b_{j,d+2} \rangle &= \frac{C}{L_l^2L_j^2}\Big[\widehat{|x|^4f} - 2X_l \cdot \widehat{|x|^2xf} + |X_l|^2\widehat{|x|^2f} - 2X_j \cdot \widehat{x|x|^2f} \end{aligned}$$

$$+4\sum_{n,m=1}^{d}(X_l)_n(X_j)_m\widehat{x_nx_mf}-2|X_l|^2X_j\cdot\widehat{xf}$$
$$+\widehat{|x|^2f}|X_j|^2-2|X_j|^2X_l\cdot\widehat{xf}+|X_l|^2|X_j|^2\widehat{f}\Big](\xi)$$

Moreover, we recall that $\mathbf{A}$ is hermitian, so the above relations allow us to obtain all

We now compute the components of the vector S. For $j,k,l,m=1,\dots,N$, let

$$\left|\begin{aligned}
C_{\Im} &:= \exp\left\{i\left(\gamma_k+\gamma_l-\gamma_m-\gamma_j\right)\right\}\\
&\quad\times\exp\left\{i\left(\beta_j\cdot X_j+\beta_m\cdot X_m-\beta_l\cdot X_l-\beta_k\cdot X_k\right)\right\}\\
&\quad\times\exp\left\{-i\left(\frac{B_k}{4L_k^2}|X_k|^2+\frac{B_l}{4L_l^2}|X_l|^2-\frac{B_m}{4L_m^2}|X_m|^2-\frac{B_j}{4L_j^2}|X_j|^2\right)\right\},\\
C_{\Re} &:= \exp\left\{-\frac{1}{2}\left(\frac{|X_k|^2}{L_k^2}+\frac{|X_l|^2}{L_l^2}+\frac{|X_m|^2}{L_m^2}+\frac{|X_j|^2}{L_j^2}\right)\right\},\\
C &:= \frac{A_kA_lA_m}{L_kL_lL_m}C_{\Im}C_{\Re},\\
\xi &:= -\left[\beta_k+\beta_l-\beta_m-\beta_j+\frac{B_k}{2L_k^2}X_k+\frac{B_l}{2L_l^2}X_l-\frac{B_m}{2L_m^2}X_m-\frac{B_j}{2L_j^2}X_j\right],\\
z &:= \frac{1}{2}\left(\frac{1}{L_k^2}+\frac{1}{L_l^2}+\frac{1}{L_m^2}+\frac{1}{L_j^2}\right)+i\left(\frac{B_k}{4L_k^2}+\frac{B_l}{4L_l^2}-\frac{B_m}{4L_m^2}-\frac{B_j}{4L_j^2}\right),\\
a &:= \frac{1}{L_k^2}X_k+\frac{1}{L_l^2}X_l+\frac{1}{L_m^2}X_m+\frac{1}{L_j^2}X_j.
\end{aligned}\right. \tag{3.13}$$

Those quantities obviously depend on the indices j,k,l and m, but for clarity we do not write explicitly these dependences since they are pretty clear. Then, for $1\le r\le d$,

$$\begin{aligned}
\langle u|u|^2,b_{j,1}\rangle &= \sum_{k,l,m}C\widehat{f}(\xi)\\
\langle u|u|^2,b_{j,r+1}\rangle &= \sum_{k,l,n}\frac{C}{L_j}\left(\widehat{x_rf}-(X_j)_r\widehat{f}\right)\\
\langle u|u|^2,b_{j,d+2}\rangle &= \sum_{k,l,m}\frac{C}{L_j^2}\left(\widehat{|x|^2f}-2X_j\cdot\widehat{xf}+|X_j|^2\widehat{f}\right).
\end{aligned}$$

We refer to Appendix D for more details. Moreover, Appendix E contains Table 1 which gives useful Fourier transforms.

Remark 3.4 (Computational complexity). Throughout this section, we have chosen

$$v_j(s_j,y_j)=e^{-\frac{1}{2}|y_j|^2}.$$

This choice was made so that the inner products involved in the application of the DFMP are easily computable in an exact way. Therefore we do not rely on numerical integration to compute the coefficients of the linear system (3.9). In particular, this shows that the computational effort required to obtain the linear system is $\mathcal{O}(N^4d+N^2(d+2)^2)$. To obtain the total complexity, we have to add the cost of computing the pseudo-inverse of the hermitian matrix $\mathbf{A}\in\mathbb{C}^{(d+2)N,(d+2)N}$, which is $O((d+2)^3N^3)$. This yields the overall computational complexity: $\mathcal{O}(N^4 d + d^3 N^3)$. In a more general setting, one could use the Hermite basis decomposition (2.8) and perform all computations exactly. This would yield more involved computations and we chose the easy way out by experimenting only with Gaussian functions, but this is completely doable.

We obtain Algorithm 2 which can be used to obtain an approximate solution to (cNLS) as a sum of bubbles, using the Strang splitting between the linear and nonlinear parts, and using an arbitrary explicit time-integrator for the nonlinear part.

Algorithm 2 Approximating a solution to (cNLS) as a sum of bubbles.

---

for Each timestep of size dt **do**
  for $j = 1, \dots, N$ **do** ▷ j denotes a bubble's index.
    Use Algorithm 1 to update the bubbles over a timestep of size $dt/2$.
    for each stage of a time-integrator **do**
      Compute the coefficients of the linear system (3.9).
      Solve the linear system (3.9) to obtain $\mathbf{E}$.
      Use (3.11) to update the parameters over a timestep whose length depends on the stage of the time-integrator.
    end for
    Use Algorithm 1 to update the bubbles over a timestep of size $dt/2$.
  end for
end for

3.2 Hamiltonian and norm conservation for the interactions

When solving (cNLS-nonLin.) via the DFMP, i.e. when solving the linear system (3.9), a Hamiltonian is conserved.

Lemma 3.1. *Let $u(t)$ be the approximation to (cNLS-nonLin.) obtained by applying the Dirac-Frenkel-MacLachlan principle, and define*

$$H_{\text{interactions}}(t) := \frac{1}{4}\langle u(t), u(t)|u(t)|^2\rangle = \frac{1}{4}\langle u(t)^2, u(t)^2\rangle.$$

Then $H_{\text{interactions}}$ is conserved, i.e.

$$\frac{\mathrm{d}}{\mathrm{d}t} H_{\text{interactions}}(t) = 0,$$

and the $\mathbb{L}^2$ norm of u is also conserved.

Proof. We have

$$H_{\text{interactions}}(t) := \frac{1}{4}\langle u(t), u(t)|u(t)|^2\rangle = \frac{1}{4}\langle u(t)^2, u(t)^2\rangle,$$

by using the Hermitian property of the inner product $\langle\cdot,\cdot\rangle$. Then,

$$\frac{\mathrm{d}}{\mathrm{d}t} H_{\text{interactions}}(t) = \frac{1}{4}\frac{\mathrm{d}}{\mathrm{d}t}\langle u(t)^2, u(t)^2\rangle$$

$$
\begin{aligned}
&= \frac{1}{4}\left\langle 2u(t)\partial_t u(t), u(t)^2\right\rangle + \frac{1}{4}\left\langle u(t)^2, 2u(t)\partial_t u(t)\right\rangle \\
&= \Re\left\langle u(t)\partial_t u(t), u(t)^2\right\rangle \\
&= \Re\left\langle \partial_t u(t), u(t)|u(t)|^2\right\rangle.
\end{aligned}
$$

By definition of $\partial_t u(t)$, we have $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$, hence we can take $f = \partial_t u(t)$ in (3.2). We obtain the following equality:

$$\langle \partial_t u(t), u(t)|u(t)|^2\rangle = \langle \partial_t u(t), i\partial_t u(t)\rangle = -i\|\partial_t u(t)\|^2.$$

Therefore,

$$\frac{\mathrm{d}}{\mathrm{d}t} H_{\text{interactions}}(t) = \Re\left(-i\|\partial_t u(t)\|^2\right) = 0.$$

Using similar ideas, we can easily show the conservation of the $\mathbb{L}^2$ norm: we obviously have $u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$, hence

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|^2 &= 2\Re\langle u(t), \partial_t u(t)\rangle = 2\Re\langle u(t), -iu(t)|u(t)|^2\rangle \\
&= 2\Re\left(i\langle |u(t)|^2, |u(t)|^2\rangle\right) = 0
\end{aligned}
$$

□

3.3 Recovering the Harmonic Oscillator equations

Suppose the family $B_{u(t)} \subset \mathbb{L}^2(\mathbb{R}^d)$ defined by (3.4) is linearly independent, and consider the equation (HO). By summing equation (2.5) over $j = 1, \ldots, N$ with $v_j(s_j, y_j) = e^{-\frac{|y_j|^2}{2}}$, and letting this sum be equal to zero, we obtain an equation of the form

$$\sum_{j=1}^{N} \left(c_{j,1}b_{j,1} + c_{j,2}b_{j,2} + \cdots + c_{j,d+1}b_{j,d+1} + c_{j,d+2}b_{j,d+2}\right) = 0. \tag{3.14}$$

Thanks to the assumption that $B_{u(t)}$ is a linearly independent family, we know that we must have

$$c_{k,1} = c_{k,2} = \cdots = c_{k,d+1} = c_{k,d+2} = 0, \qquad k = 1, \ldots, (d+2)N. \tag{3.15}$$

This yields exactly the system of equations (2.10). In other words, the DFMP approach gives the same equations as those given in Section 2.3 when $B_{u(t)}$ is a linearly independent family. However, our approach as described in Section 2.3 allows to solve them exactly and not only numerically with some numerical time-integrator.

Finally, if the family $B_{u(t)}$ is linearly dependent, then we cannot write equation (3.15) anymore, hence the DFMP approach in the linear case fails. Our approach avoids this issue by naturally imposing conditions (3.15) (which are the same as (2.6)).

4 Numerical examples

In this section we will assess the efficiency of the Bubbles approach with the Dirac-Frenkel-MacLachlan approach against a spectral method in the two-dimensional case.

4.1 Spectral scheme

We start by discussing the spectral method we shall use to compare with the results of Algorithm 2. We refer to [For96] for a general introduction to spectral methods for the Schrödinger equation, and to [ABB13] for grid-based schemes applied to the Gross-Pitaevskii equation.

We now present a method which can be understood as the application of [BCL21] to a simpler equation, namely the Harmonic Oscillator. We use a splitting method to simulate the linear part (HO), and thanks to [Ber20, AB21] we have:

$$\begin{aligned} e^{-it(-\Delta+|x|^2)} &= e^{-\frac{1}{2}\tanh(it)|x|^2} e^{\frac{1}{2}\sinh(2it)\Delta_x} e^{-\frac{1}{2}\tanh(it)|x|^2} \\ &= e^{-\frac{i}{2}\tan(t)|x|^2} e^{\frac{i}{2}\sin(2t)\Delta_x} e^{-\frac{i}{2}\tan(t)|x|^2}. \end{aligned} \tag{4.1}$$

We can cite [JMS11] which also presents a spectral method based on the Fourier transform with time splitting, however the above method is different in that (4.1) is exact and hence we do not have any time-splitting error.

The first and third exponentials on the RHS are straightforward to compute on a grid. For the second one, we use a Fourier transform: $e^{\frac{i}{2}\sin(2t)\Delta_x}$ is the propagator of the following equation:

$$\partial_t \psi = i\cos(2t)\Delta_x \psi.$$

By using a Fourier transform, we get

$$\partial_t \mathcal{F}(\psi)(\xi) = i\cos(2t)\mathcal{F}\left(\Delta_x \psi\right)(\xi) = -i\cos(2t)|\xi|^2 \mathcal{F}\left(\psi\right)(\xi).$$

Hence,

$$\mathcal{F}(\psi(t,\cdot))(\xi) = e^{-\frac{i}{2}\sin(2t)|\xi|^2}\mathcal{F}(\psi(0,\cdot))(\xi).$$

The RHS exponential is straightforward to compute in the Fourier space. Hence, an exact-time spectral approximation of the solution to (HO) is given by Algorithm 3. From this, it is easy to obtain an algorithm which simulates (cNLS) with interactions. It consists in using a Strang splitting method on (cNLS), by splitting the linear part (HO) and the nonlinear part (cNLS-nonLin.). The linear part is approximated via Algorithm 3, and the computation of interactions is explicit thanks to the fact that $|u(t,x)|^2$ does not depend on time (see e.g. [Fao12, Sect. 2.2]). This fully describes Algorithm 4.

Of course, in pratical applications one is not able to define a grid over $\mathbb{R}^d$. Hence, Algorithms 3 and 4 have to be modified by defining Grid as a discretization of a finite-volume subset of $\mathbb{R}^d$, typically a product of intervals in each dimension. For all of our numerical examples, this will $[-15, 15] \times [-15, 15]$, discretized using $N_x \times N_y$ points. In order to have an easily computable FFT, one has to use a spatial uniform grid, which then defines the Fourier Grid. Special care has to be paid when choosing the number of points: if we have Fourier frequencies larger than the *Nyquist frequency*, then we will observe a phenomenon known as *aliasing*. This may not be problematic for the Harmonic Oscillator (HO) depending on the initial condition, but will eventually become an issue when simulating (cNLS) because it involves interactions and hence an infinite number of frequencies. Moreover, by using a FFT-based algorithm we implicitly impose periodic boundary conditions.

Algorithm 3 Spectral solver for (HO), with an exact time resolution for each splitting step.

Discretize the initial data η on a Grid $\subset \mathbb{R}^d$.
for Each timestep of size Δt **do**
  for $x \in$ GRID **do** ▷ $x \in \mathbb{R}^d$.
    Multiply $\eta(x)$ by $e^{-\frac{i}{2}\tan(\Delta t)|x|^2}$.
  end for
  Apply a FFT to η. ▷ FFT: Fast Fourier Transform.
  for $\xi \in$ FOURIER GRID **do** ▷ $\xi \in \mathbb{R}^d$.
    Multiply $\mathcal{F}(\eta)(\xi)$ by $e^{-\frac{i}{2}\sin(2\Delta t)|\xi|^2}$.
  end for
  Apply an inverse FFT to $\mathcal{F}(\eta)$.
  for $x \in$ GRID **do**
    Multiply $\eta(x)$ by $e^{-\frac{i}{2}\tan(\Delta t)|x|^2}$.
  end for
end for

Algorithm 4 Spectral solver for (cNLS), with a Strang Splitting method.

Discretize the initial data η on a Grid $\subset \mathbb{R}^d$.
for Each timestep of size Δt **do**
  Use Algorithm 3 with a stepsize $\Delta t/2$.
  for $x \in$ GRID **do** ▷ Add interactions.
    Multiply $\eta(x)$ by $e^{-i\,\Delta t\,|\eta(x)|^2}$.
  end for
  Use Algorithm 3 with a stepsize $\Delta t/2$.
end for

4.2 Discretization into a sum of Bubbles

We need to decompose any arbitrary function into a finite sum of N bubbles. A solution to this question has been proposed in [QY10], but it involves integrals over the whole phase space, which is something we want to avoid.

We could also use a nonlinear least squares approach, but our experimental results showed that it tends to yield spread out Gaussians, which may present huge overlaps between them. The overlaps cause issues with the DFMP, for instance a blow-up of the conservative quantities. This has been observed during our experiments but the results are not reported in this paper. The issue of discretizing an arbitrary function into a sum of bubbles without too much overlap is not the main concern of this paper, hence we will use a visual trial-and-error discretization. Another possible way of discretizing the initial data is outlined in [AKLP22]. Finally, if we do not restrict ourselves to Gaussian functions and allow general Hermite functions, then the discretization simply consists in projecting the initial condition onto this basis, and truncating the highest modes if necessary.

4.3 Observables

In order to compare the bubbles scheme against the spectral method, we compare them in absence of interactions, i.e. on the Harmonic Oscillator (HO), as well as in the presence of nonlinear interactions, i.e. on (cNLS). We showed in Lemma 2.1 the conservation of some quantities for (HO) and (cNLS), we will focus on mass, energy and momentum. When computing the observables for the spectral solution, we noted that the approximation of the gradient using finite differences with periodic boundary conditions yielded very rough results while the gradient approximation using the Fast Fourier Transform gave more accurate results. We use the latter approximation in the Figures of Section 4.4. In the case of bubbles, we compute every integral by hand thanks to the assumption $v(s,y) = e^{-\frac{|y|^2}{2}}$, some details are given in Appendix F. When reporting the results in the following log-plots, all values with an amplitude smaller than 10^{-16} were set to be equal to 10^{-16}.

For all of the results shown, the spectral scheme is supplied with the exact initial condition and not a projection on the grid of the bubbles discretization.

4.4 Results

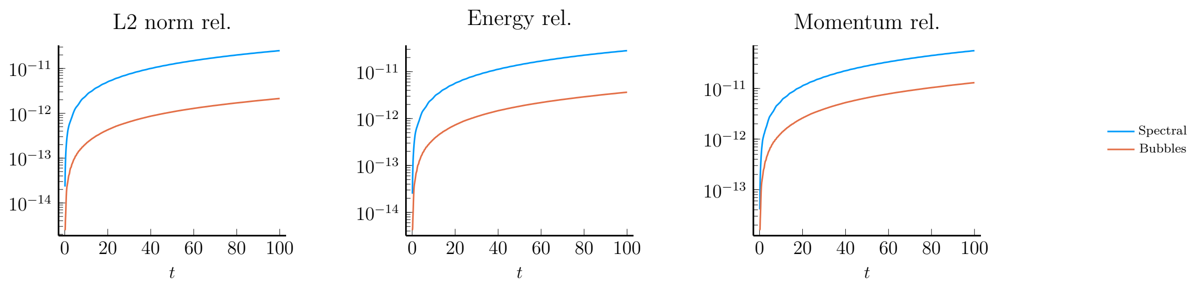
We consider examples adapted from [BJM03].

4.4.1 Test case 1: Zero phase initial data

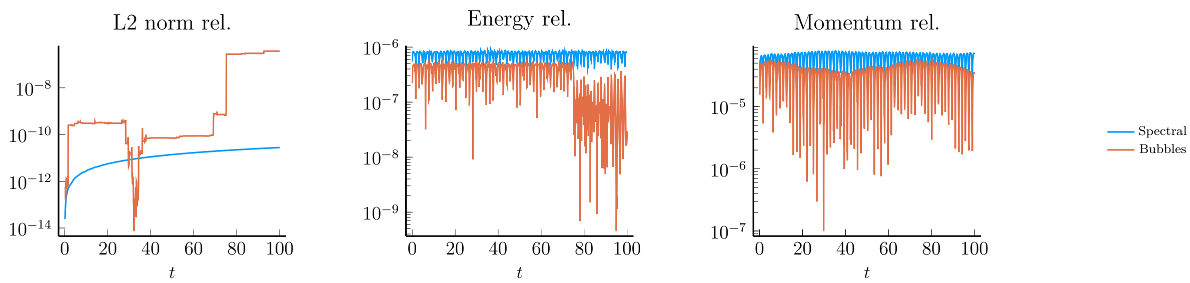
The initial condition reads

$$\psi(t=0,x) = \pi e^{-\frac{|x-\mu_1|^2}{2}} + 2e^{-\frac{|x-\mu_2|^2}{2}}, \quad x \in \mathbb{R}^2, \quad \mu_1 = (0,2),\ \mu_2 = (1,0). \tag{4.2}$$

The results are displayed in Figure 1. The solution approximated with the DFMP approach globally outperforms the spectral method on both the Harmonic Oscillator and the cubic NonLinear Schrödinger equations. On the Harmonic Oscillator, the solution obtained with the Bubbles scheme is about one order of magnitude better than the spectral

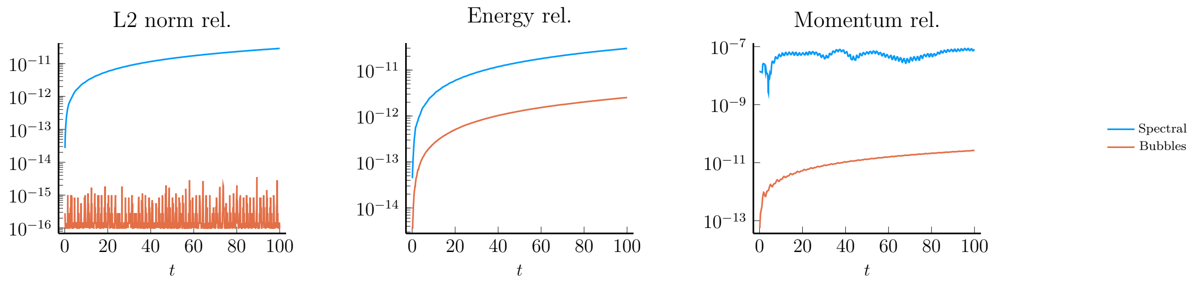


(a) Approximate solution to the Harmonic Oscillator (HO).

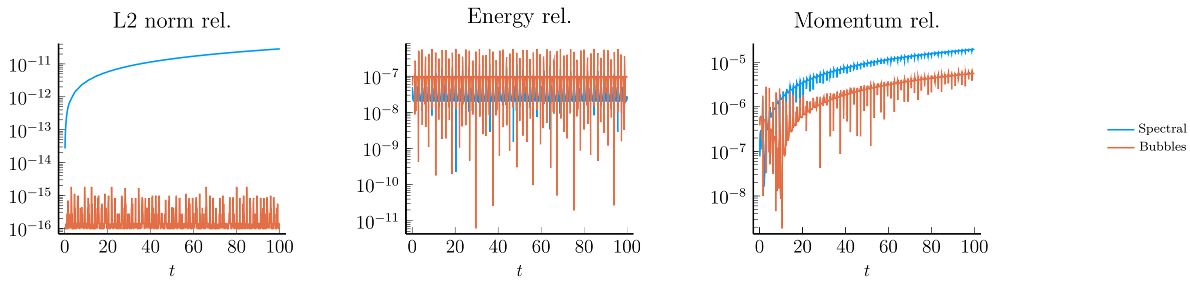


(b) Approximate solution to the Schrödinger equation (cNLS) using DFMP Algorithm.

Figure 1: Test case 1. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 129$.



(a) Approximate solution to the Harmonic Oscillator (HO).



(b) Approximate solution to the Schrödinger equation (cNLS) using DFMP Algorithm.

Figure 2: Test case 2. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 129$.

scheme. When we compare them on (cNLS), i.e. when adding interactions, the $\mathbb{L}^2$ norm is better conserved for the spectral scheme, but the other conservative quantities are better conserved on a long time for the Bubbles scheme.

The "jumps" in the DFMP approach may be explained by an ill-conditioned Gram matrix, which would then yield a very rough approximation of the modulation parameters.

4.4.2 Test case 2: Weak interactions

The initial condition reads

$$\psi(t=0,x) = e^{-|x-\mu_3|^2} e^{i\cosh|x-\mu_3|}, \quad x \in \mathbb{R}^2, \quad \mu_3 = (1,1). \tag{4.3}$$

The approximation of this function as a sum of bubbles is pretty straightforward: we know that for x small, $\cosh x \approx 1 + \frac{x^2}{2}$, hence

$$\psi(t=0,x) \approx e^{-|x-\mu_3|^2} e^{i+i\frac{|x-\mu_3|^2}{2}}, \quad x \in \mathbb{R}^2.$$

The results are displayed in Figure 2. This example shows the performance of the DFMP approach in its most efficient setting: it only has one bubble. This explains the very good conservation results obtained: the Bubbles scheme outperforms the spectral scheme on both (HO) and (cNLS), except for the energy on (cNLS). However, even in this case, the error of the DFMP method remains generally less than one order of magnitude larger than the error from the spectral method.

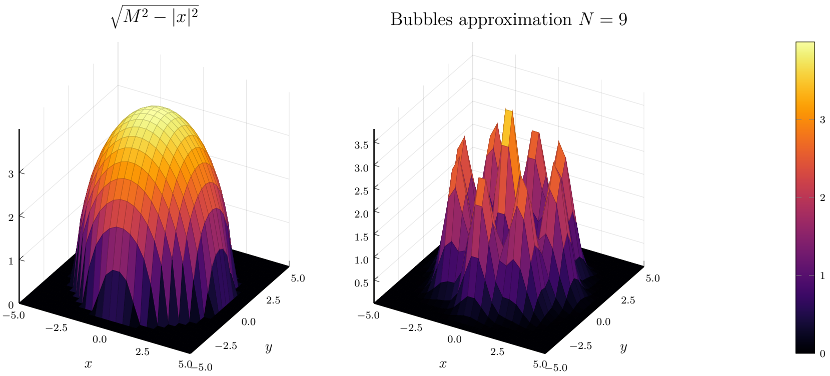


Figure 3: Approximation of $x \mapsto \sqrt{M^2 - |x|^2}$ as a sum of bubbles

4.4.3 Test case 3: Strong interactions

The initial condition reads

$$\psi(t=0,x) = \begin{cases} \sqrt{M^2 - |x|^2} e^{i \cosh \sqrt{x_1^2 + x_2^2}}, & |x|^2 < M^2 \\ 0 & \text{otherwise} \end{cases}, \quad M = 4. \tag{4.4}$$

We apply the same approximation for the complex exponential as previously explained, and use a "visual trial-and-error" discretization of the square root. It yields a number of $N = 9$ bubbles. We emphasize the fact that this discretization may be far from being the best one achievable, however the process of discretizing an arbitrary function into a sum of bubbles is not the main concern of this paper. The discretization of the initial square root is given in Figure 3.

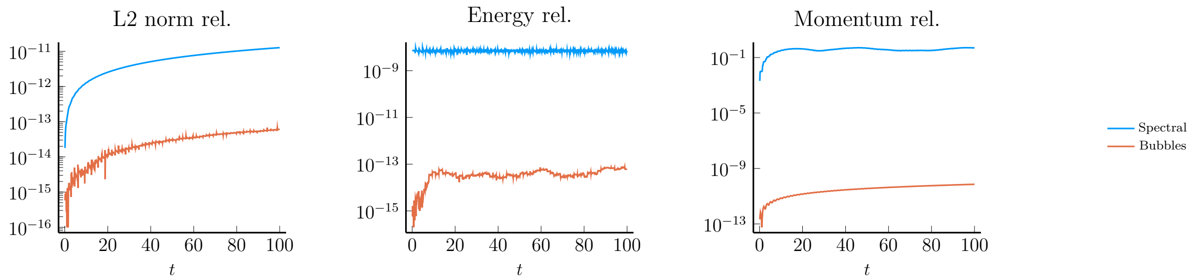
The results are displayed in Figure 4. This example is by far the most interesting of the three test cases presented in this paper, because it shows that with the discretization given in Figure 3 the conservation properties are pretty good for the Bubbles scheme, even when there are a lot of interactions between bubbles. The spectral scheme is globally outperformed by the Bubbles scheme, except for the $\mathbb{L}^2$ norm in the presence of interactions, which is better conserved by the spectral scheme. Even in this case, the conservation of this quantity with the DFMP is relatively correct.

The "jumps" in the relative evolution of conservative quantities may be explained by an ill-conditioned Gram matrix in DFMP. It also has to be noted that if the discretization presents too much overlap between the Gaussian functions, then the DFMP approach fails and the conservative quantities blow up: this has been observed with other discretizations of the same initial data, and is not reported here.

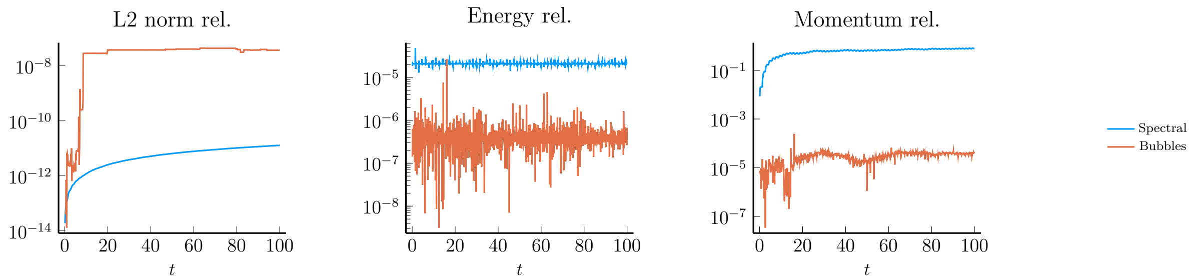
5 Conclusion

We presented in this work an approach based on recent results from [FR20]. It allows to solve exactly the Harmonic Oscillator (HO) for initial functions that can be represented as a sum of modulated functions (the *bubbles*), for a certain kind of modulation.

In this context we focused on a particular subclass of such functions, modulated Hermite functions, which have the advantage of allowing explicit computations. This is



(a) Approximate solution to the Harmonic Oscillator (HO).



(b) Approximate solution to the Schrödinger equation (cNLS) using DFMP Algorithm.

Figure 4: Test case 3. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 129$.

particularly interesting since we do not have to rely on any sort of discretization of the phase space, which is usually the main computational burden in numerical simulations. We obtain an algorithm which yields an exact solution as soon as the initial data is a sum of modulated Hermite functions. If we consider an arbitrary initial function, it suffices to project it into onto the Hermite basis and to perform analytical time-evolution. Moreover, the algorithm only relies on a small number of parameters whose time-evolution is explicit, making it very fast and computationally efficient.

We also extended the results from [FR20] by allowing cubic interactions, at the cost of approximating the solution to (cNLS-nonLin.) via the Dirac-Frenkel-MacLachlan principle. We then only considered modulated Gaussian functions, because they allowed us to easily perform explicit computations and to obtain a numerical algorithm whose computational complexity is $\mathcal{O}(N^4 d + N^3 d^3)$. Here d is the dimension and N is the number of bubbles. The most critical parameter is N, which corresponds roughly to the precision of the discretization when considering arbitrary initial data. For any given function, the higher N, the better we can approximate it as a sum of modulated Gaussian functions. We then have a clear trade-off between the speed of the algorithm and the precision of the discretization. The bubble algorithm globally outperforms on the numerical test cases a spectral method combined with time splitting, where each splitting step is solved exactly.

As a final note, any grid-based method is inherently bound to a finite subset of $\mathbb{R}^d$ to which we have to add boundary conditions, while the bubble approach does not have such restrictions. We emphasize the fact that the algorithm presented extends in a straightforward manner when dealing with complex modulated Hermite functions.

Acknowledgements

The authors would like to thank J. Bernier for spotting an abnormal behavior in the spectral method and for his help in fixing it. EF and YLH were sponsored by the Centre Henri Lebesgue, program ANR-11-LABX-0020-0. EF and PR were sponsored by the Inria Associated team *Bubbles*.

Appendix A   Proof of Lemma 2.1

We will need the following result, known as the Pohozaev identity.

Lemma A.1 (Pohozaev Identity)**.** *Let $x \in \mathbb{R}^d$, and $f \in H^1(\mathbb{R}^d)$ such that $xf \in \mathbb{L}^2(\mathbb{R}^d)$. Then*

$$\int \Delta f \overline{\left(\frac{d}{2} f + x \cdot \nabla f\right)} dx = - \int |\nabla f|^2 dx. \tag{A.1}$$

Proof. By density, we only need to prove equation (A.1) for $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$, where $\mathcal{C}_c^\infty(\mathbb{R}^d)$ denotes the space of infinitely smooth functions with compact support in $\mathbb{R}^d$. Let

$$f_\lambda(x) := \lambda^{\frac{d}{2}} f(\lambda x),$$

then

$$\int |\nabla f_\lambda|^2 dx = \lambda^2 \int |\nabla f|^2 dx.$$

Differentiating this identity with respect to λ and evaluating the result at $\lambda = 1$ yields

$$\int \nabla f \cdot \overline{\nabla \left(\frac{d}{2} f + x \cdot \nabla f\right)} dx = \int |\nabla f|^2 dx.$$

We integrate by parts the LHS, and obtain (A.1). □

Now turn to the proof of Lemma 2.1.

Mass conservation:

$$\begin{aligned}
\partial_t \|\psi\|_{\mathbb{L}^2}^2 &= \partial_t \int |\psi|^2 = 2\Re \int \bar{\psi} \partial_t \psi = 2\Re \int -i\bar{\psi} \left(-\mu\Delta\psi + \mu|x|^2\psi + \lambda|\psi|^2\psi\right) \\
&= 2\Re \int -i \left(\mu\bar{\psi}\Delta\psi + \mu|x|^2|\psi|^2 + \lambda|\psi|^4\right) = 2\mu\Re \int -i\bar{\psi}\Delta\psi \\
&= 2\mu\Re \int i|\nabla\psi|^2 = 0.
\end{aligned}$$

Energy conservation:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} E_{\mu,\lambda} &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t} \left\langle -\mu\Delta\psi + \mu|x|^2\psi + \frac{\lambda}{2}|\psi|^2\psi, \psi \right\rangle \\
&= \frac{1}{2}\left(-2\mu\Re\langle\Delta\psi, \partial_t\psi\rangle + 2\mu\Re\langle|x|^2\psi, \partial_t\psi\rangle + 4\Re\left\langle \frac{\lambda}{2}|\psi|^2\psi, \partial_t\psi \right\rangle\right) \\
&= \Re\left(i\langle\partial_t\psi, \partial_t\psi\rangle\right) = 0.
\end{aligned}$$

For the momentum, we compute

$$\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int |x|^2|\psi|^2 &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\langle|x|^2\psi, \psi\rangle = \Re\langle|x|^2\psi, \partial_t\psi\rangle = \Re\langle|x|^2\psi, i\mu\Delta\psi - i\mu|x|^2\psi - i\lambda|\psi|^2\psi\rangle \\
&= \mu\Im\langle|x|^2\psi, \Delta\psi\rangle = \mu\Im\int |x|^2\psi\Delta\bar{\psi} = -\mu\Im\int \nabla\bar{\psi}\cdot\nabla\left(|x|^2\psi\right) \\
&= -\mu\Im\int \nabla\bar{\psi}\cdot 2x\psi - \mu\Im\int \nabla\bar{\psi}\cdot\nabla\psi|x|^2 = -2\mu\Im\int x\cdot\nabla\bar{\psi}\psi \\
&= 2\mu\Im\int x\cdot\nabla\psi\bar{\psi}, \qquad \text{(A.2)}
\end{aligned}$$

and

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im\int x\cdot\nabla\psi\bar{\psi} = \frac{1}{2}\Im\int \left(x\cdot\nabla\partial_t\psi\bar{\psi} + x\cdot\nabla\psi\partial_t\bar{\psi}\right).$$

An integration by parts gives

$$\int x\cdot\nabla\phi\psi = -\int \phi\nabla\cdot(x\psi) = -\int \phi\left(\psi d + x\cdot\nabla\psi\right),$$

hence

$$\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im\int x\cdot\nabla\psi\bar{\psi} &= \frac{1}{2}\Im\int\left(-\partial_t\psi\left(\bar{\psi}d + x\cdot\nabla\bar{\psi}\right) + x\cdot\nabla\psi\partial_t\bar{\psi}\right) \\
&= \frac{1}{2}\Im\int\left(-\partial_t\psi\bar{\psi}d - \partial_t\psi x\cdot\nabla\bar{\psi} + \partial_t\bar{\psi}x\cdot\nabla\psi\right) \\
&= \frac{1}{2}\Im\int\left(-\partial_t\psi\bar{\psi}d + 2i\Im\left[\partial_t\bar{\psi}x\cdot\nabla\psi\right]\right)
\end{aligned}$$

$$= -\frac{d}{2}\Im \int \partial_t \psi \bar{\psi} + \Im \int \partial_t \bar{\psi} x \cdot \nabla \psi.$$

Recall the equation satisfied by ψ:

$$\partial_t \psi = i\mu\Delta\psi - i\mu|x|^2\psi - i\lambda|\psi|^2\psi,$$

therefore

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im \int x \cdot \nabla\psi\bar{\psi} &= -\frac{d}{2}\Im \int i\left[\mu\Delta\psi - \mu|x|^2\psi - \lambda|\psi|^2\psi\right]\bar{\psi} \\ &\quad + \Im \int i\left[-\mu\Delta\bar{\psi} + \mu|x|^2\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi.\end{aligned}$$

We have

$$-\frac{d}{2}\Im \int i\left[\mu\Delta\psi - \mu|x|^2\psi - \lambda|\psi|^2\psi\right]\bar{\psi} = \frac{d}{2}\int \left[\mu|\nabla\psi|^2 + \mu|x|^2|\psi|^2 + \lambda|\psi|^4\right],$$

and

$$\Im \int i\left[-\mu\Delta\bar{\psi} + \mu|x|^2\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi = \Re \int \left[-\mu\Delta\bar{\psi} + \mu|x|^2\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi.$$

Moreover,

$$\begin{aligned}\int |x|^2\bar{\psi}x \cdot \nabla\psi &= -\int \psi\nabla \cdot \left(x|x|^2\bar{\psi}\right) = -\int \psi\left(d|x|^2\bar{\psi} + 2|x|^2\bar{\psi} + x|x|^2 \cdot \nabla\bar{\psi}\right) \\ \iff \int |x|^2\bar{\psi}x \cdot \nabla\psi + \overline{\int |x|^2\bar{\psi}x \cdot \nabla\psi} &= -\int \psi\left(d|x|^2\bar{\psi} + 2|x|^2\bar{\psi}\right) \\ \iff \Re \int |x|^2\bar{\psi}x \cdot \nabla\psi &= -\int \psi\left(\frac{d}{2}|x|^2\bar{\psi} + |x|^2\bar{\psi}\right).\end{aligned}$$

Finally,

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im \int x \cdot \nabla\psi\bar{\psi} &= \frac{d}{2}\int \left[\mu|\nabla\psi|^2 + \mu|x|^2|\psi|^2 + \lambda|\psi|^4\right] \\ &\quad + \Re \int \left[-\mu\Delta\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi - \mu\int \psi\left(\frac{d}{2}|x|^2\bar{\psi} + |x|^2\bar{\psi}\right) \\ &= \frac{d}{2}\int \left[\mu|\nabla\psi|^2 + \lambda|\psi|^4\right] + \Re \int \left[-\mu\Delta\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi - \mu\int |x|^2|\psi|^2 \\ &= \frac{d}{2}\mu\int |\nabla\psi|^2 - \mu\int |x|^2|\psi|^2 + \frac{d}{2}\lambda\int |\psi|^4 + \Re \int \left[-\mu\Delta\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi\end{aligned}$$

We are in the two-dimensional case $d = 2$, hence

$$\begin{aligned}\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im \int x \cdot \nabla\psi\bar{\psi} &= \int \mu|\nabla\psi|^2 - \mu\int |x|^2|\psi|^2 + \lambda\int |\psi|^4 + \Re \int \left[-\mu\Delta\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi \\ &= 2E_\lambda + \frac{\lambda}{2}\int |\psi|^4 - 2\mu\int |x|^2|\psi|^2 + \Re \int \left[-\mu\Delta\bar{\psi} + \lambda|\psi|^2\bar{\psi}\right] x \cdot \nabla\psi.\end{aligned}$$

Moreover,

$$\int |\psi|^2\bar{\psi}x \cdot \nabla\psi = -\int \psi\nabla \cdot \left(|\psi|^2\bar{\psi}x\right)$$

$$
\begin{aligned}
&= -\int \psi \left(2\Re\left(\bar\psi \nabla \psi\right)\cdot \bar\psi x + |\psi|^2 \nabla\bar\psi\cdot x + d|\psi|^2\bar\psi\right)\\
&= -\int \left(2\Re\left(\bar\psi \nabla \psi\right)\cdot |\psi|^2 x + \psi|\psi|^2 \nabla\bar\psi\cdot x + 2|\psi|^4\right)
\end{aligned}
$$

$$
\iff 2\Re\int |\psi|^2\bar\psi x\cdot\nabla\psi = -2\Re\int \bar\psi\nabla\psi\cdot|\psi|^2 x - 2\int|\psi|^4
$$

$$
\iff \Re\int |\psi|^2\bar\psi x\cdot\nabla\psi = -\frac{1}{2}\int|\psi|^4,
$$

Finally,

$$
\begin{aligned}
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im\int x\cdot\nabla\psi\bar\psi &= 2E_\lambda + \frac{\lambda}{2}\int|\psi|^4 - 2\mu\int|x|^2|\psi|^2 - \mu\Re\int\Delta\bar\psi x\cdot\nabla\psi - \frac{\lambda}{2}\int|\psi|^4\\
&= 2E_\lambda - 2\mu\int|x|^2|\psi|^2 - \mu\Re\int\Delta\bar\psi x\cdot\nabla\psi
\end{aligned}
$$

We then use the Pohozaev identity (A.1) in dimension $d=2$, which yields

$$
\Re\left(\int x\cdot\nabla\psi\Delta\bar\psi\right) = 0.
$$

Therefore,

$$
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Im\int x\cdot\nabla\psi\bar\psi = 2E_{\mu,\lambda} - 2\mu\int|x|^2|\psi|^2.
$$

From the conservation of the energy E_λ and equation (A.2),

$$
\frac{\mathrm{d}^2}{\mathrm{d}t^2}\Im\int x\cdot\nabla\psi\bar\psi = -16\mu^2\Im\int x\cdot\nabla\psi\bar\psi.
$$

Hence, the conservation laws

$$
\begin{aligned}
&\frac{1}{16}\left(\frac{\mathrm{d}}{\mathrm{d}t}\left[\Im\int x\cdot\nabla\psi\bar\psi\right]\right)^2 + \mu^2\left(\Im\int x\cdot\nabla\psi\bar\psi\right)^2\\
&= \left(E_{\mu,\lambda} - \mu\|x\psi\|_{\mathbb{L}^2}^2\right)^2 + \mu^2\left(\Im\int x\cdot\nabla\psi\bar\psi\right)^2
\end{aligned}
$$

For the non radial conservation law:

$$
\frac{\mathrm{d}}{\mathrm{d}t}\Im\int\partial_j\psi\bar\psi = -2\Im\int\partial_t\psi\overline{\partial_j\psi} = 2\Re\int i\partial_t\psi\overline{\partial_j\psi} = 2\mu\int|x|^2\Re\left(\psi\overline{\partial_j\psi}\right) = -2\mu\int x_j|\psi|^2,
$$

owing to the facts that integrations by parts yield

$$
-\Re\int\Delta\psi\partial_j\bar\psi = \Re\int\partial_j\psi\Delta\bar\psi,
$$

and

$$
2\Re\int|\psi|^2\psi\partial_j\bar\psi = \int|\psi|^2\partial_j|\psi|^2 = -\int|\psi|^2\partial_j|\psi|^2 \implies \Re\int|\psi|^2\psi\partial_j\bar\psi = 0.
$$

We also have

$$
\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int x_j|\psi|^2 = \Re\int x_j\partial_t\psi\bar\psi = \Im\int x_j i\partial_t\psi\bar\psi = \mu\Im\int -\Delta\psi x_j\bar\psi = \mu\Im\int\partial_j\psi\bar\psi.
$$

Hence the relations

$$\left| \begin{array}{l} \frac{\mathrm{d}}{\mathrm{d}t} \int x_j |\psi|^2 = 2\mu \Im \int \partial_j \psi \bar{\psi} \\ \frac{\mathrm{d}}{\mathrm{d}t} \Im \int \partial_j \psi \bar{\psi} = -2\mu \int x_j |\psi|^2, \end{array} \right.$$

which have the conservation law

$$\mathcal{P}_j = \frac{1}{4} \left(\Im \int \partial_j \psi \bar{\psi} \right)^2 + \mu^2 \left(\int x_j |\psi|^2 \right)^2 .$$

Appendix B Proof of Lemma 2.2

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

$$X_i = \sqrt{2a_i(0)} \sin(2t + \theta_i(0)) \quad \text{and} \quad \beta_i = \sqrt{2a_i(0)} \cos(2t + \theta_i(0)) \qquad i = 1, \dots, d,$$

are solutions.

For the (k, B) part we use the method of generating functions, described e.g. in [HLW06, 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:

$$B = 2\sqrt{e^{4k}\mathcal{E} - e^{8k} - 1}. \tag{B.1}$$

This equality holds for $e^{4k} \in [e^{4k_0}, e^{4k_1}]$, where e^{4k_0}, e^{4k_1} are the reals roots of the polynomial $-z^2 + \mathcal{E}z - 1$,

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

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 $[k_0, k]$:

$$S(k, \mathcal{E}) = 2 \int_{k_0}^{k} \sqrt{e^{4z}\mathcal{E} - e^{8z} - 1} dz.$$

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

$$\phi = \frac{\partial S}{\partial \mathcal{E}}(k, \mathcal{E}) = \int_{k_0}^{k} \frac{e^{4z}}{\sqrt{e^{4z}\mathcal{E} - e^{8z} - 1}} dz.$$

We have

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = \frac{e^{4k} k_t}{\sqrt{e^{4k} - e^{8k} - 1}} = \frac{-e^{4k} \partial_B \mathcal{E}}{\frac{B}{2}} = \frac{-e^{-4k} \frac{B}{2} e^{4k}}{\frac{B}{2}} = -1.$$

We now proceed to obtaining an explicit expression for ψ:

$$\begin{aligned}
\phi &= \int_{k_0}^{k} \frac{e^{4z}}{\sqrt{e^{4z}\mathcal{E} - e^{8z} - 1}} dz = \frac{1}{4}\int_{e^{4k_0}}^{e^{4k}} \frac{1}{\sqrt{\mathcal{E}u - u^2 - 1}} du \\
&= \frac{1}{4\sqrt{\frac{\mathcal{E}^2}{4} - 1}} \int_{e^{4k_0}}^{e^{4k}} \frac{1}{\sqrt{1 - \left(\frac{u - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right)^2}} du \\
&= \frac{1}{4}\int_{\frac{e^{4k_0} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}}^{\frac{e^{4k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}} \frac{1}{\sqrt{1 - u^2}} du.
\end{aligned}$$

Recall the definition (B.2) of k_0, which yields

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

Therefore,

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

We want the angle variable to lie in $[0, 2\pi]$ 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,

$$\xi = \arcsin\left(\frac{e^{4k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right) + \frac{\pi}{2} \in [0, \pi], \tag{B.3}$$

and hence

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

We obtain

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

With this formula, we have

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

and (B.1) becomes

$$\begin{aligned} B &= 2\sqrt{\mathcal{E}e^{4k} - e^{8k} - 1} = 2\sqrt{4he^{4k} - (e^{4k})^2 - 1} = 2\sqrt{(4h^2-1)\sin^2(\xi)} \\ &= 2\sin(\xi)\sqrt{4h^2-1}, \end{aligned}$$

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

We can now integrate the equations for A, and γ. The first one is

$$A_t = \frac{AB}{2}(d-2)e^{-4k}.$$

From the expressions we just obtained we get

$$A_t = A(d-2)\frac{\sin(\xi)\sqrt{4h^2-1}}{2h - \cos(\xi)\sqrt{4h^2-1}}.$$

The solution to this equation is of the form

$$A(t) = A(0)\exp\left\{(d-2)\int_0^t \frac{\sin(\xi(\sigma))\sqrt{4h(\sigma)^2-1}}{2h(\sigma) - \cos(\xi(\sigma))\sqrt{4h(\sigma)^2-1}}\mathrm{d}\sigma\right\}.$$

Moreover, we know that $\sigma \mapsto h(\sigma)$ is constant, and that $\xi(\sigma) = \xi(0) - 4\sigma$. Hence we have to solve

$$A(t) = A(0)\exp\left\{(d-2)\int_0^t \frac{\sin(\xi(0)-4\sigma)\sqrt{4h(0)^2-1}}{2h(0) - \cos(\xi(0)-4\sigma)\sqrt{4h(0)^2-1}}\mathrm{d}\sigma\right\}.$$

One can easily check that we have the following equality:

$$\begin{aligned} &\int_0^t \frac{\sin(\xi(0)-4\sigma)\sqrt{4h(0)^2-1}}{2h(0) - \cos(\xi(0)-4\sigma)\sqrt{4h(0)^2-1}}\mathrm{d}\sigma \\ &= -\frac{1}{4}\left[\log\left(2h(t) - \cos(\xi(t))\sqrt{4h(t)^2-1}\right) - \log\left(2h(0) - \cos(\xi(0))\sqrt{4h(0)^2-1}\right)\right]. \end{aligned}$$

Note that, unless $h(0) = \frac{1}{2}$ or $h(t) = \frac{1}{2}$, these quantities are well-defined since $2h(\sigma) > \sqrt{4h(\sigma)^2 - 1}, \sigma \in \{0, t\}$. Thus, we obtain

$$\begin{aligned} A(t) &= A(0)e^{\frac{2-d}{4}\left[\log\left(2h(t)-\cos(\xi(t))\sqrt{4h(t)^2-1}\right) - \log\left(2h(0)-\cos(\xi(0))\sqrt{4h(0)^2-1}\right)\right]} \\ &= C\left(2h(0) - \cos(\xi(0)-4t)\sqrt{4h(0)^2-1}\right)^{\frac{2-d}{4}}, \end{aligned}$$

where we defined $C := A(0)\left(2h(0) - \cos(\xi(0))\sqrt{4h(0)^2-1}\right)^{\frac{d-2}{4}}$. We recognize here the expressions for $L(0)^2$ and $L(t)^2$.

Let us finally turn to the expression for $\gamma(t)$. We proceed to the direct integration of γ_t. We have

$$\gamma(t) - \gamma(0) = \int_0^t \dot{\gamma}(\tau)d\tau = \int_0^t \left[|\beta(\tau)|^2 - |X(\tau)|^2\right]d\tau$$

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

where the last equality has been obtained using (2.14).

Finally, we calculate the evolution of the time $s(t)$ in term of the original time t. Owing to the expression of $L(t)$ we obtained earlier,

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

Recall the following trigonometric identity:

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

hence

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

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

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

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

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

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,

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

Hence

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

$$+\frac{1}{2}\arctan\left((c_1+c_2)\tan\left(\frac{\xi(0)}{2}\right)\right)+m_t\frac{\pi}{2}.$$

Appendix C Proof of Lemma 2.3

Proof. We have $a_i(0)=\frac{1}{2}\left(X_i(0)^2+\beta_i(0)^2\right), i=1,\dots,d$. If $a_i(0)>0$ we can define $\theta_i(0)$ as $\theta_i(0)=\arctan\left(\frac{X_i(0)}{\beta_i(0)}\right)$. Otherwise, if $a_i(0)=0$, then we recall that $a(t)=a(0)$ and hence – whatever $\theta(0)$ – we have $X_i(t)=0$ and $\beta_i(t)=0$. Therefore, in the case $a_i(0)=0$, the exact value of $\theta_i(0)$ does not change the behavior of $t\mapsto(X_i(t),\beta_i(t))$.

For the (L,B) part,

$$L(0)^2-2h(0)=-\cos(\xi(0))\sqrt{4h(0)^2-1},$$

hence

$$(L(0)^2-2h(0))^2=L(0)^4-4L(0)^2h(0)+4h(0)^2=\cos(\xi(0))^2\left(4h(0)^2-1\right).$$

We also have

$$\left(\frac{B(0)}{2}\right)^2=\frac{B(0)^2}{4}=\sin(\xi(0))^2\left(4h(0)^2-1\right).$$

Then,

$$L(0)^4-4L(0)^2h(0)+4h(0)^2+\frac{B(0)^2}{4}=4h(0)^2-1,$$

that is

$$4L(0)^2h(0)=L(0)^4+\frac{B(0)^2}{4}+1.$$

We deduce that $h(0),L(0)\neq 0$, and therefore

$$h(0)=\frac{L(0)^4+\frac{B(0)^2}{4}+1}{4L(0)^2}.$$

Note that $h(0)$ is bounded from below by $\frac{1}{2}$. Indeed,

$$\begin{aligned}
&L(0)^4-2L(0)^2+1+\frac{B(0)^2}{4}=\left(L(0)^2-1\right)^2+\frac{B(0)^2}{4}\geq 0\\
\iff& L(0)^4+1+\frac{B(0)^2}{4}\geq 2L(0)^2\\
\iff& h(0)\geq\frac{1}{2}.
\end{aligned}$$

From this we also get that $h(0)=\frac{1}{2}\iff L(0)^2=1$ and $B(0)=0$.

If $h(0)>\frac{1}{2}$, we have

$$\begin{cases}2h(0)-L(0)^2=\cos(\xi(0))\sqrt{4h(0)^2-1}\\ \dfrac{B(0)}{2}=\sin(\xi(0))\sqrt{4h(0)^2-1},\end{cases}\implies\frac{B(0)/2}{2h(0)-L(0)^2}=\tan(\xi(0)),$$

hence

$$\xi(0) = \arctan\left(\frac{B(0)/2}{2h(0) - L(0)^2}\right).$$

Otherwise, in the case $h(0) = \frac{1}{2}$, the value of $\xi(0)$ is not rigourously defined. However, as previously, the exact value of $\xi(0)$ is not important because $h(t) = h(0) = \frac{1}{2}$, which means that $L(t)^2 = 1$ and $B(t) = 0$. Therefore, in the case $h(0) = \frac{1}{2}$, the mapping $t \mapsto (L(t), B(t))$ does not depend on the value of $\xi(0)$. Finally, since the mapping $t \mapsto L(t)$ does not depend on $\xi(0)$ in the case $h(0) = \frac{1}{2}$, we also have that $t \mapsto A(t)$ does not depend on the exact value of $\xi(0)$, thanks to the expression of $A(t) = A(0)\left(L(t)/L(0)\right)^{\frac{2-d}{2}}$.

Finally, it remains to show that if $a_i(0) = 0$, $i \in \{1, \ldots, d\}$ or $h(0) = \frac{1}{2}$, then the behavior of the mappings $t \mapsto \gamma(t)$ and $t \mapsto s(t)$ do not depend on the exact value of $\theta_i(0)$, $i \in \{1, \ldots, d\}$ or $\xi(0)$. The exact formulae for $\gamma(t)$ and $s(t)$ are:

$$\begin{aligned}
\gamma(t) &= \gamma(0) + \sum_{l=1}^{d} \frac{a_l(0)}{2}\left[\sin(2\theta_l(t)) - \sin(2\theta_l(0))\right] \\
s(t) &= \frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(0)}{2} - 2t\right)\right) \\
&\quad - \frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(0)}{2}\right)\right) - m_t\frac{\pi}{2}
\end{aligned}$$

It is clear that if $a_i(0) = 0$ then $\gamma(t)$ does not depend on $\theta_i(0)$ nor $\theta_i(t)$, $i \in \{1, \ldots, d\}$. If $h(0) = \frac{1}{2}$, then

$$2h(0) + \sqrt{4h(0)^2 - 1} = 1,$$

so that

$$\begin{aligned}
&\frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(0)}{2} - 2t\right)\right) \\
&\qquad - \frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2 - 1}\right)\tan\left(\frac{\xi(0)}{2}\right)\right) - m_t\frac{\pi}{2} \\
&= \frac{1}{2}\arctan\left(\tan\left(\frac{\xi(t)}{2}\right)\right) - \frac{1}{2}\arctan\left(\tan\left(\frac{\xi(0)}{2}\right)\right) - m_t\frac{\pi}{2}.
\end{aligned}$$

Since $\arctan : \mathbb{R} \mapsto \left(-\frac{\pi}{2}, \frac{\pi}{2}\right]$, we 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 we have

$$\begin{aligned}
&\frac{1}{2}\arctan\left(\tan\left(\frac{\xi(t)}{2}\right)\right) - \frac{1}{2}\arctan\left(\tan\left(\frac{\xi(0)}{2}\right)\right) - m_t\frac{\pi}{2} \\
&= \frac{1}{2}\widetilde{\frac{\xi(t)}{2}} - \frac{1}{2}\widetilde{\frac{\xi(0)}{2}} - m_t\frac{\pi}{2} \\
&= \frac{1}{2}\frac{\xi(t)}{2} - (m_0 - m_t)\frac{\pi}{2} - \frac{1}{2}\left(\frac{\xi(0)}{2} - m_0\pi\right) - m_t\frac{\pi}{2} \\
&= \frac{1}{2}\left(\frac{\xi(t)}{2} - \frac{\xi(0)}{2}\right) = -t.
\end{aligned}$$

This shows that, in the case $h(0) = \frac{1}{2}$, the mapping $t \mapsto \gamma(t)$ does not depend on the value chosen for the ill-defined quantity $\xi(0)$. □

Appendix D Computing the coefficients of the linear system (3.9)

D.1 Coefficients of the matrix A

$\langle b_{l,1}, b_{j,1}\rangle$.

$$\langle b_{l,1}, b_{j,1}\rangle = e^{i\gamma_l - i\gamma_j}\int_{\mathbb{R}^d} e^{iL_l\beta_l\cdot\frac{x-X_l}{L_l} - i\frac{B_l}{4}\left|\frac{x-X_l}{L_l}\right|^2} e^{-\frac{1}{2}\left|\frac{x-X_l}{L_l}\right|^2} \times e^{-iL_j\beta_j\cdot\frac{x-X_j}{L_j} + i\frac{B_j}{4}\left|\frac{x-X_j}{L_j}\right|^2} e^{-\frac{1}{2}\left|\frac{x-X_j}{L_j}\right|^2} dx$$

$$= e^{i(\gamma_l-\gamma_j)}\int_{\mathbb{R}^d} e^{i\beta_l\cdot(x-X_l) - i\beta_j\cdot(x-X_j)} e^{-\frac{2+iB_l}{4}\left|\frac{x-X_l}{L_l}\right|^2} e^{-\frac{2-iB_j}{4}\left|\frac{x-X_j}{L_j}\right|^2} dx$$

$$= e^{i(\gamma_l-\gamma_j) - \frac{2+iB_l}{4L_l^2}|X_l|^2 - \frac{2-iB_j}{4L_j^2}|X_j|^2 - i\beta_l\cdot X_l + i\beta_j\cdot X_j} \times \int_{\mathbb{R}^d} e^{i(\beta_l-\beta_j)\cdot x} e^{-\frac{2+iB_l}{4L_l^2}(|x|^2 - 2x\cdot X_l)} e^{-\frac{2-iB_j}{4L_j^2}(|x|^2-2x\cdot X_j)} dx$$

$$= e^{i(\gamma_l-\gamma_j) - \frac{2+iB_l}{4L_l^2}|X_l|^2 - \frac{2-iB_j}{4L_j^2}|X_j|^2 - i\beta_l\cdot X_l + i\beta_j\cdot X_j} \times \int_{\mathbb{R}^d} e^{i(\beta_l - \beta_j + \frac{B_l}{2L_l^2}X_l - \frac{B_j}{2L_j^2}X_j)\cdot x} e^{x\cdot\left(\frac{1}{L_l^2}X_l + \frac{1}{L_j^2}X_j\right)} e^{-\left(\frac{2+iB_l}{4L_l^2} + \frac{2-iB_j}{4L_j^2}\right)|x|^2} dx$$

Let

$$\left|\begin{aligned} & z := \frac{2+iB_l}{4L_l^2} + \frac{2-iB_j}{4L_j^2}, \\ & a := \frac{X_l}{L_l^2} + \frac{X_j}{L_j^2}, \\ & \xi := \frac{B_j}{2L_j^2}X_j + \beta_j - \frac{B_l}{2L_l^2}X_l - \beta_l, \\ & C = \exp\left\{i(\gamma_l-\gamma_j) - \frac{2+iB_l}{4L_l^2}|X_l|^2 - \frac{2-iB_j}{4L_j^2}|X_j|^2 - i\beta_l\cdot X_l + i\beta_j\cdot X_j\right\}, \end{aligned}\right. \tag{D.1}$$

and $f(x) := e^{-z|x|^2 + a\cdot x}$. Then

$$\langle b_{l,1}, b_{j,1}\rangle = C\int_{\mathbb{R}^d} e^{-i\xi\cdot x} f(x)dx = C\widehat{f}(\xi)$$

$\langle b_{l,n+1}, b_{j,1}\rangle$, $1 \le n \le d$.

$$\begin{aligned}\langle b_{l,n+1}, b_{j,1}\rangle &= C\int_{\mathbb{R}^d}\frac{(x-X_l)_n}{L_l}e^{-i\xi\cdot x}f(x)dx \\ &= \frac{C}{L_l}\left(\widehat{xf}_n - (X_l)_n\widehat{f}\right)(\xi)\end{aligned}$$

$\langle b_{l,d+2}, b_{j,1}\rangle$

$$\begin{aligned}\langle b_{l,d+2}, b_{j,1}\rangle &= C\int_{\mathbb{R}^d} e^{-i\xi\cdot x} f(x)\frac{|x-X_l|^2}{L_l^2}dx \\ &= \frac{C}{L_l^2}\int_{\mathbb{R}^d} e^{-i\xi\cdot x} f(x)\left(|x|^2 - 2x\cdot X_l + |X_l|^2\right)dx \\ &= \frac{C}{L_l^2}\left(\widehat{|x|^2 f} - 2X_l\cdot\widehat{xf} + |X_l|^2\widehat{f}\right)(\xi)\end{aligned}$$

<u>$\langle b_{l,n+1}, b_{j,m+1}\rangle$, $1\le n,m\le d$.</u>

$$\begin{aligned}\langle b_{l,n+1}, b_{j,m+1}\rangle &= C\int_{\mathbb{R}^d}\frac{x_n-(X_l)_n}{L_l}\frac{x_m-(X_j)_m}{L_j}e^{-i\xi\cdot x}f(x)dx \\ &= \frac{C}{L_jL_l}\int_{\mathbb{R}^d}(x_n-(X_l)_n)(x_m-(X_j)_m)e^{-i\xi\cdot x}f(x)dx \\ &= \frac{C}{L_jL_l}\int_{\mathbb{R}^d}\left[x_nx_m - x_n(X_j)_m - x_m(X_l)_n + (X_l)_n(X_j)_m\right] \\ &\qquad\qquad \times e^{-i\xi\cdot x}f(x)dx \\ &= \frac{C}{L_jL_l}\left[\widehat{x_nx_mf} - (X_l)_n\widehat{x_mf} - (X_j)_m\widehat{x_nf} + (X_l)_n(X_j)_m\widehat{f}\right](\xi).\end{aligned}$$

<u>$\langle b_{l,d+2}, b_{j,m+1}\rangle$, $1\le m\le d$.</u>

$$\begin{aligned}&\langle b_{l,d+2}, b_{j,m+1}\rangle \\ &= C\int_{\mathbb{R}^d} e^{-i\xi\cdot x}e^{-z|x|^2+a\cdot x}\frac{|x-X_l|^2}{L_l^2}\frac{x_m-(X_j)_m}{L_j}dx \\ &= \frac{C}{L_l^2L_j}\int_{\mathbb{R}^d} e^{-i\xi\cdot x}e^{-z|x|^2+a\cdot x}\left(|x|^2-2x\cdot X_l+|X_l|^2\right)\left(x_m-(X_j)_m\right)dx \\ &= \frac{C}{L_l^2L_j}\Big[\widehat{x_m|x|^2f} - 2X_l\cdot\widehat{x_mxf} + |X_l|^2\widehat{x_mf} \\ &\qquad -(X_j)_m\widehat{|x|^2f} + 2(X_j)_mX_l\cdot\widehat{xf} - |X_l|^2(X_j)_m\widehat{f}\Big](\xi).\end{aligned}$$

<u>$\langle b_{l,d+2}, b_{j,d+2}\rangle$</u>

$$\begin{aligned}\langle b_{l,d+2}, b_{j,d+2}\rangle &= C\int_{\mathbb{R}^d} e^{-i\xi\cdot x}e^{-z|x|^2+a\cdot x}\frac{|x-X_l|^2}{L_l^2}\frac{|x-X_j|^2}{L_j^2}dx \\ &= \frac{C}{L_l^2L_j^2}\int_{\mathbb{R}^d} e^{-i\xi\cdot x}e^{-z|x|^2+a\cdot x}\left(|x|^2-2x\cdot X_l+|X_l|^2\right) \\ &\qquad\qquad\times\left(|x|^2-2x\cdot X_j+|X_j|^2\right)dx \\ &= \frac{C}{L_l^2L_j^2}\int_{\mathbb{R}^d} e^{-i\xi\cdot x}e^{-z|x|^2+a\cdot x}\Big(|x|^4 - 2|x|^2x\cdot X_l + |X_l|^2|x|^2 \\ &\qquad\qquad - 2(x\cdot X_j)|x|^2 + 4(x\cdot X_l)(x\cdot X_j) - 2(x\cdot X_j)|X_l|^2\end{aligned}$$

$$
\begin{aligned}
&\quad + |x|^2|X_j|^2 - 2(x\cdot X_l)|X_j|^2 + |X_l|^2|X_j|^2\Big)\,dx \\
&= \frac{C}{L_l^2 L_j^2}\Big[\widehat{|x|^4 f} - 2(X_l+X_j)\cdot\widehat{|x|^2 x f} + \left(|X_l|^2+|X_j|^2\right)\widehat{|x|^2 f} \\
&\quad + 4\widehat{(x\cdot X_l)(x\cdot X_j) f} - 2\left(|X_l|^2X_j + |X_j|^2X_l\right)\cdot\widehat{xf} \\
&\quad + |X_l|^2|X_j|^2\widehat{f}\Big](\xi)
\end{aligned}
$$

Moreover,

$$
\begin{aligned}
(x\cdot X_l)(x\cdot X_j) &= \left(\sum_{n=1}^d x_n (X_l)_n\right)\left(\sum_{m=1}^d x_m (X_j)_m\right) \\
&= \sum_{n,m=1}^d (X_l)_n (X_j)_m x_n x_m,
\end{aligned}
$$

Hence

$$
\widehat{(x\cdot X_l)(x\cdot X_j) f} = \sum_{n,m=1}^d (X_l)_n (X_j)_m \widehat{x_n x_m f}.
$$

D.2 Coefficients of the vector of interactions S

$\langle u|u|^2, b_{j,1}\rangle$

$$
\langle u|u|^2, b_{j,1}\rangle = \sum_{k,l,m} \frac{A_k A_l A_m}{L_k L_l L_m}\left\langle e^{i\Gamma_k + i\Gamma_l - i\Gamma_m} e^{-\frac{|y_k|^2+|y_l|^2+|y_m|^2}{2}}, e^{i\Gamma_j} e^{-\frac{1}{2}|y_j|^2}\right\rangle
$$

We recall the previously defined notations:

$$
\left|
\begin{aligned}
y_k &= \frac{x-X_k}{L_k}, \\
\Gamma_k(x) &= \gamma_k + \beta_k\cdot(x-X_k) - \frac{B_k}{4L_k^2}|x-X_k|^2.
\end{aligned}
\right.
$$

Then,

$$
\begin{aligned}
&-\frac{1}{2}\left(|y_k|^2+|y_l|^2+|y_m|^2+|y_j|^2\right) = -\frac{1}{2L_k^2}|x-X_k|^2 - \frac{1}{2L_l^2}|x-X_l|^2 - \frac{1}{2L_m^2}|x-X_m|^2 \\
&\qquad\qquad - \frac{1}{2L_j^2}|x-X_j|^2 \\
&= -\frac{1}{2}\left(\frac{1}{L_k^2}+\frac{1}{L_l^2}+\frac{1}{L_m^2}+\frac{1}{L_j^2}\right)|x|^2 + \left(\frac{1}{L_k^2}X_k + \frac{1}{L_l^2}X_l + \frac{1}{L_m^2}X_m + \frac{1}{L_j^2}X_j\right)\cdot x \\
&\quad - \frac{1}{2}\left(\frac{|X_k|^2}{L_k^2}+\frac{|X_l|^2}{L_l^2}+\frac{|X_m|^2}{L_m^2}+\frac{|X_j|^2}{L_j^2}\right),
\end{aligned}
$$

and

$$
(\Gamma_k + \Gamma_l - \Gamma_m - \Gamma_j)
$$

$$= \gamma_k + \beta_k \cdot (x - X_k) - \frac{B_k}{4L_k^2}|x - X_k|^2 + \gamma_l + \beta_l \cdot (x - X_l) - \frac{B_l}{4L_l^2}|x - X_l|^2$$
$$- \gamma_m - \beta_m \cdot (x - X_m) + \frac{B_m}{4L_m^2}|x - X_m|^2 - \gamma_j - \beta_j \cdot (x - X_j) + \frac{B_j}{4L_j^2}|x - X_j|^2$$
$$= (\gamma_k + \gamma_l - \gamma_m - \gamma_j) + (\beta_j \cdot X_j + \beta_m \cdot X_m - \beta_l \cdot X_l - \beta_k \cdot X_k)$$
$$- \left(\frac{B_k}{4L_k^2}|X_k|^2 + \frac{B_l}{4L_l^2}|X_l|^2 - \frac{B_m}{4L_m^2}|X_m|^2 - \frac{B_j}{4L_j^2}|X_j|^2 \right)$$
$$+ x \cdot \left(\beta_k + \beta_l - \beta_m - \beta_j + \frac{B_k}{2L_k^2}X_k + \frac{B_l}{2L_l^2}X_l - \frac{B_m}{2L_m^2}X_m - \frac{B_j}{2L_j^2}X_j \right)$$
$$- \left(\frac{B_k}{4L_k^2} + \frac{B_l}{4L_l^2} - \frac{B_m}{4L_m^2} - \frac{B_j}{4L_j^2} \right) |x|^2$$

Define

$$\begin{aligned}
C_{\Im} &:= \exp\left\{ i \left(\gamma_k + \gamma_l - \gamma_m - \gamma_j \right) \right\} \\
&\quad \times \exp\left\{ i \left(\beta_j \cdot X_j + \beta_m \cdot X_m - \beta_l \cdot X_l - \beta_k \cdot X_k \right) \right\} \\
&\quad \times \exp\left\{ -i \left(\frac{B_k}{4L_k^2}|X_k|^2 + \frac{B_l}{4L_l^2}|X_l|^2 - \frac{B_m}{4L_m^2}|X_m|^2 - \frac{B_j}{4L_j^2}|X_j|^2 \right) \right\} \\
C_{\Re} &:= \exp\left\{ -\frac{1}{2} \left(\frac{|X_k|^2}{L_k^2} + \frac{|X_l|^2}{L_l^2} + \frac{|X_m|^2}{L_m^2} + \frac{|X_j|^2}{L_j^2} \right) \right\} \\
C &:= \frac{A_k A_l A_m}{L_k L_l L_m} C_{\Im} C_{\Re} \\
\xi &:= - \left[\beta_k + \beta_l - \beta_m - \beta_j + \frac{B_k}{2L_k^2}X_k + \frac{B_l}{2L_l^2}X_l - \frac{B_m}{2L_m^2}X_m - \frac{B_j}{2L_j^2}X_j \right] \\
z &:= \frac{1}{2} \left(\frac{1}{L_k^2} + \frac{1}{L_l^2} + \frac{1}{L_m^2} + \frac{1}{L_j^2} \right) + i \left(\frac{B_k}{4L_k^2} + \frac{B_l}{4L_l^2} - \frac{B_m}{4L_m^2} - \frac{B_j}{4L_j^2} \right) \\
a &:= \frac{1}{L_k^2}X_k + \frac{1}{L_l^2}X_l + \frac{1}{L_m^2}X_m + \frac{1}{L_j^2}X_j
\end{aligned}$$

and $f(x) := e^{-z|x|^2 + a \cdot x}$. Then

$$\langle u|u|^2, b_{j,1} \rangle = \sum_{k,l,m} C \widehat{f}(\xi). \tag{D.2}$$

<u>$\langle u|u|^2, b_{j,r+1} \rangle$, $r = 1, \ldots, d$</u>

$$\begin{aligned}
&\langle u|u|^2, b_{j,r+1} \rangle \\
&= \sum_{k,l,m} \frac{A_k A_l A_m}{L_k L_l L_m} \left\langle e^{i\Gamma_k + i\Gamma_l - i\Gamma_m} e^{-\frac{|y_k|^2 + |y_l|^2 + |y_m|^2}{2}}, e^{i\Gamma_j} e^{-\frac{1}{2}|y_j|^2} \frac{x_r - (X_j)_r}{L_j} \right\rangle \\
&= \sum_{k,l,m} \frac{C}{L_j} \left(\widehat{x_r f} - (X_j)_r \widehat{f} \right).
\end{aligned}$$

<u>$\langle u|u|^2, b_{j,d+2} \rangle$</u>

$h(x)$	$\widehat{h}(\xi)/e^{-\frac{(\xi+ia)\cdot(\xi+ia)}{4z}}$
f	$\left(\frac{\pi}{z}\right)^{\frac{d}{2}}$
xf	$-i\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\frac{\xi+ia}{2z}$
$x_m x_n f$	$-\frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_n+ia_n)(\xi_m+ia_m)$
$x_m^2 f$	$\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[1-\frac{(\xi_m+ia_m)^2}{2z}\right]$
$\|x\|^2 f$	$\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[d-\frac{\|\xi\|^2+2ia\cdot\xi-\|a\|^2}{2z}\right]$
$x_m\|x\|^2 f$	$-\frac{i}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_m+ia_m)\left[d+2-\frac{\|\xi\|^2+2ia\cdot\xi-\|a\|^2}{2z}\right]$
$x_m^2 x_n^2 f$	$\frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)\left(1-\frac{(\xi_m+ia_m)^2}{2z}\right)$
$x_m^4 f$	$\frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[3-6\frac{(\xi_m+ia_m)^2}{2z}+\frac{(\xi_m+ia_m)^4}{4z^2}\right]$

Table 1: Fourier Transform of some polynomials in $x=(x_1,\dots,x_d)\in\mathbb{R}^d$ multiplied by $f(x)=e^{-z|x|^2+a\cdot x}$, $z\in\mathbb{C},\Re(z)>0, a\in\mathbb{R}^d$.

$$\begin{aligned}
&\langle u|u|^2, b_{j,d+2}\rangle \\
&= \sum_{k,l,m}\frac{A_kA_lA_m}{L_kL_lL_m}\left\langle e^{i\Gamma_k+i\Gamma_l-i\Gamma_m}e^{-\frac{|y_k|^2+|y_l|^2+|y_m|^2}{2}}, e^{i\Gamma_j}e^{-\frac{1}{2}|y_j|^2}\left|\frac{x-X_j}{L_j}\right|^2\right\rangle \\
&= \sum_{k,l,m}\frac{C}{L_j^2}\left(\widehat{|x|^2f}-2X_j\cdot\widehat{xf}+|X_j|^2\widehat{f}\right).
\end{aligned}$$

Appendix E Fourier transforms of Gaussians

Lemma E.1 (Fourier transform of complex Gaussians). *Let $z\in\mathbb{C}$, $\Re(z)\geq 0$. Then,*

$$\mathcal{F}\left(e^{-z|\cdot|^2}\right)(\xi)=\left(\frac{\pi}{z}\right)^{\frac{d}{2}}e^{-\frac{|\xi|^2}{4z}},\quad \xi\in\mathbb{R}^d. \tag{E.1}$$

More generally, let $z=z_1+iz_2\in\mathbb{C}$, $z_1,z_2\in\mathbb{R}$, $z_1>0$, $a\in\mathbb{R}^d$ and

$$f:\ x\in\mathbb{R}^d\mapsto\exp\left(-z|x|^2+a\cdot x\right)\in\mathbb{C}, \tag{E.2}$$

then we have the Fourier transforms given by Table 1.

Proof. For the sake of clarity, for $\xi, a \in \mathbb{R}^d$ and $z \in \mathbb{C}$, let

$$E(\xi, a, z) := \exp\left\{-\frac{|\xi|^2 + 2ia\cdot\xi - |a|^2}{4z}\right\} = \exp\left\{-\frac{(\xi + ia)\cdot(\xi + ia)}{4z}\right\}.$$

$\underline{\widehat{f}.}$

We have

$$-z|x|^2 + a\cdot x = -z\left|x - \frac{a}{2z_1}\right|^2 - i\frac{z_2 a}{z_1}\cdot x + \frac{z|a|^2}{4z_1^2}.$$

Recall the following usual properties on Fourier transform:

$$\widehat{f(x-a)} = \widehat{f}(\xi)e^{-ia\cdot\xi}, \quad \widehat{fe^{-ia\cdot x}} = \widehat{f}(\xi + a).$$

Let

$$g(x) = e^{-z\left|x - \frac{a}{2z_1}\right|^2},$$

then

$$\hat{g}(\xi) = \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{-\frac{|\xi|^2}{4z} - \frac{ia\cdot\xi}{2z_1}}$$

and

$$f(x) = g(x)e^{-\frac{iz_2}{z_1}a\cdot x + \frac{z|a|^2}{4z_1^2}}.$$

Hence,

$$\begin{aligned}
\widehat{f}(\xi) &= e^{\frac{z|a|^2}{4z_1^2}}\,\hat{g}\left(\xi + \frac{z_2}{z_1}a\right) = \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{\frac{z|a|^2}{4z_1^2}} e^{-\frac{1}{4z}\left|\xi + \frac{z_2}{z_1}a\right|^2 - \frac{ia}{2z_1}\cdot\left(\xi + \frac{z_2}{z_1}a\right)} \\
&= \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{\frac{z|a|^2}{4z_1^2} - \frac{1}{4z}\left(|\xi|^2 + 2\frac{z_2}{z_1}a\cdot\xi + \frac{z_2^2}{z_1^2}|a|^2\right) - \frac{ia\cdot\xi}{2z_1} - \frac{i|a|^2 z_2}{2z_1^2}} \\
&= \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{-\frac{|\xi|^2}{4z} + (a\cdot\xi)\left(-\frac{z_2}{2zz_1} - \frac{i}{2z_1}\right) + |a|^2\left(\frac{z}{4z_1^2} - \frac{z_2^2}{4zz_1^2} - \frac{iz_2}{2z_1^2}\right)} \\
&= \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{-\frac{|\xi|^2}{4z} - \frac{a\cdot\xi}{2zz_1}[z_2 + i(z_1 + iz_2)] + \frac{|a|^2}{4zz_1^2}\left[(z_1 + iz_2)^2 - z_2^2 - 2iz_2(z_1 + iz_2)\right]} \\
&= \left(\frac{\pi}{z}\right)^{\frac{d}{2}} e^{-\frac{|\xi|^2}{4z} - i\frac{a\cdot\xi}{2z} + \frac{|a|^2}{4z}} \\
&= \left(\frac{\pi}{z}\right)^{\frac{d}{2}} E(\xi, a, z).
\end{aligned}$$

$\underline{\widehat{xf}.}$

$$\begin{aligned}
\widehat{xf}(\xi) &= i\nabla_\xi \hat{f} = i\nabla_\xi\left[\left(\frac{\pi}{z}\right)^{\frac{d}{2}} E(\xi, a, z)\right] = i\left(\frac{\pi}{z}\right)^{\frac{d}{2}} E(\xi, a, z)\left[-\frac{\xi}{2z} - \frac{ia}{2z}\right] \\
&= -i\left(\frac{\pi}{z}\right)^{\frac{d}{2}} \frac{\xi + ia}{2z} E(\xi, a, z).
\end{aligned}$$

$\widehat{x_m^2 f}$, $m = 1, \dots, d$.

$$\begin{aligned}\widehat{x_m^2 f}(\xi) &= i\partial_{\xi_m}\left(\widehat{xf}\right)_m = i\partial_{\xi_m}\left[-i\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\frac{(\xi+ia)_m}{2z}E(\xi,a,z)\right]\\ &= \frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[E(\xi,a,z)+(\xi_m+ia_m)\,E(\xi,a,z)\left(-\frac{\xi_m}{2z}-\frac{ia_m}{2z}\right)\right]\\ &= \frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[1-\frac{(\xi_m+ia_m)^2}{2z}\right]E(\xi,a,z).\end{aligned}$$

$\widehat{x_m x_n f}$, $m, n = 1, \dots, d$, $n \neq m$.

$$\begin{aligned}\widehat{x_m x_n f}(\xi) &= i\partial_{\xi_m}\left(\widehat{xf}\right)_n = i\partial_{\xi_m}\left[-i\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\frac{\xi_n+ia_n}{2z}E(\xi,a,z)\right]\\ &= \frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_n+ia_n)\left[-\frac{\xi_m+ia_m}{2z}\right]E(\xi,a,z)\\ &= -\frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_n+ia_n)\,(\xi_m+ia_m)\,E(\xi,a,z).\end{aligned}$$

$\widehat{|x|^2 f}$.

$$\begin{aligned}\widehat{|x|^2 f}(\xi) &= \widehat{x_1^2 f}(\xi)+\cdots+\widehat{x_d^2 f}(\xi)\\ &= \frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[d-\frac{(\xi_1+ia_1)^2+\cdots+(\xi_d+ia_d)^2}{2z}\right]E(\xi,a,z)\\ &= \frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[d-\frac{|\xi|^2+2ia\cdot\xi-|a|^2}{2z}\right]E(\xi,a,z).\end{aligned}$$

$\widehat{x_m|x|^2 f}$, $m = 1, \dots, d$.

$$\begin{aligned}&\widehat{x_m|x|^2 f}(\xi)\\ &= i\partial_{\xi_m}\left[\widehat{|x|^2 f}(\xi)\right] = i\partial_{\xi_m}\left[\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(d-\frac{|\xi|^2+2ia\cdot\xi-|a|^2}{2z}\right)E(\xi,a,z)\right]\\ &= \frac{i}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[-2\frac{\xi_m+ia_m}{2z}+\left(d-\frac{|\xi|^2+2ia\cdot\xi-|a|^2}{2z}\right)\left(-\frac{\xi_m+ia_m}{2z}\right)\right]E(\xi,a,z)\\ &= -\frac{i}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_m+ia_m)\left[d+2-\frac{|\xi|^2+2ia\cdot\xi-|a|^2}{2z}\right]E(\xi,a,z).\end{aligned}$$

$\underline{\widehat{x_m^3 f},\ m = 1, \dots, d.}$

$$\begin{aligned}
\widehat{x_m^3 f}(\xi) &= i\partial_{\xi_m}\left[\widehat{x_m^2 f}(\xi)\right] = i\partial_{\xi_m}\left[\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_m+ia_m)^2}{2z}\right)E(\xi,a,z)\right]\\
&= \frac{i}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[-2\frac{\xi_m+ia_m}{2z}+\left(-\frac{\xi_m+ia_m}{2z}\right)\left(1-\frac{(\xi_m+ia_m)^2}{2z}\right)\right]E(\xi,a,z)\\
&= -\frac{i}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_m+ia_m)\left[3-\frac{(\xi_m+ia_m)^2}{2z}\right]E(\xi,a,z)\\
&= -\frac{i}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[3(\xi_m+ia_m)-\frac{(\xi_m+ia_m)^3}{2z}\right]E(\xi,a,z).
\end{aligned}$$

$\underline{\widehat{x_m x_n^2 f},\ m, n = 1, \dots, d,\ n \neq m.}$

$$\begin{aligned}
\widehat{x_m x_n^2 f}(\xi) &= i\partial_{\xi_m}\left(\widehat{x_n^2 f}\right) = i\partial_{\xi_m}\left[\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)E(\xi,a,z)\right]\\
&= -\frac{i}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)\frac{\xi_m+ia_m}{2z}E(\xi,a,z).
\end{aligned}$$

$\underline{\widehat{x_m^4 f},\ m = 1, \dots, d.}$

$$\begin{aligned}
&\widehat{x_m^4 f}(\xi)\\
&= i\partial_{\xi_m}\left[\widehat{x_m^3 f}(\xi)\right] = i\partial_{\xi_m}\left[-\frac{i}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(3(\xi_m+ia_m)-\frac{(\xi_m+ia_m)^3}{2z}\right)E(\xi,a,z)\right]\\
&= \frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[3-3\frac{(\xi+ia_m)^2}{2z}+\left(3(\xi_m+ia_m)-\frac{(\xi_m+ia_m)^3}{2z}\right)\left(-\frac{\xi_m+ia_m}{2z}\right)\right]E(\xi,a,z)\\
&= \frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[3-6\frac{(\xi_m+ia_m)^2}{2z}+\frac{(\xi_m+ia_m)^4}{4z^2}\right]E(\xi,a,z).
\end{aligned}$$

$\underline{\widehat{x_m^2 x_n^2 f},\ m = 1, \dots, d,\ n \neq m.}$

$$\begin{aligned}
\widehat{x_m^2 x_n^2 f}(\xi) &= i\partial_{\xi_m}\left(\widehat{x_m x_n^2 f}\right)_n = i\partial_{\xi_m}\left[-\frac{i}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)\frac{\xi_m+ia_m}{2z}E(\xi,a,z)\right]\\
&= \frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)\partial_{\xi_m}\left[(\xi_m+ia_m)E(\xi,a,z)\right]\\
&= \frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left(1-\frac{(\xi_n+ia_n)^2}{2z}\right)\left(1-\frac{(\xi_m+ia_m)^2}{2z}\right)E(\xi,a,z).
\end{aligned}$$

□

Appendix F Miscellaneous computations

We provide in this section some miscellaneous computations, which hold in dimension $d = 2$ as long as $v_j(s_j, y_j) = e^{-\frac{|y_j|^2}{2}}$, $j = 1, \dots, N$.

F.1 Conservative quantities in dimension $d = 2$

We give the explicit expressions for the conservative quantities involved in Lemma 2.1, in the two-dimensional case.

The $\mathbb{L}^2$ norm of a sum of N bubbles is given by

$$\|u\|_{\mathbb{L}^2}^2 = \sum_{k,l=1}^{N} \frac{A_k A_l}{L_k L_l} \langle b_{k,1}, b_{l,1} \rangle.$$

The energy of a sum of bubbles is given by

$$E_{\mu,\lambda} = \frac{\mu}{2} \left\langle -\Delta u + |x|^2 u, u \right\rangle + \frac{\lambda}{4} \left\langle |u|^2 u, u \right\rangle = E_{\mu,0} + E_{0,\lambda} = \mu E_{1,0} + \lambda E_{0,1}.$$

We have

$$2E_{1,0} = \langle Hu, u \rangle = \langle -\Delta u, u \rangle + \langle |x|^2 u, u \rangle = \sum_{j,k=1}^{N} \langle \nabla_x u_j, \nabla_x u_k \rangle + \sum_{j,k=1}^{N} \langle |x|^2 u_j, u_k \rangle.$$

Furthermore,

$$\begin{aligned}
\langle \nabla_x u_j, \nabla_x u_k \rangle &= \frac{A_j A_k}{L_j L_k} \left\langle \left(i\beta_j - \frac{2 + iB_j}{2L_j} y_j \right) b_{j,1}, \left(i\beta_k - \frac{2 + iB_k}{2L_k} y_k \right) b_{k,1} \right\rangle \\
&= \frac{A_j A_k}{L_j L_k} \left\{ \beta_j \cdot \beta_k \langle b_{j,1}, b_{k,1} \rangle + i \frac{2 + iB_j}{2L_j} \beta_k \cdot \begin{pmatrix} \langle b_{j,2}, b_{k,1} \rangle \\ \langle b_{j,3}, b_{k,1} \rangle \end{pmatrix} \right. \\
&\qquad - i \frac{2 - iB_k}{2L_k} \beta_j \cdot \begin{pmatrix} \langle b_{j,1}, b_{k,2} \rangle \\ \langle b_{j,1}, b_{k,3} \rangle \end{pmatrix} \\
&\qquad \left. + \frac{2 + iB_j}{2L_j} \frac{2 - iB_k}{2L_k} \left(\langle b_{j,2}, b_{k,2} \rangle + \left\langle b_{(j,3}, b_{k,3} \right\rangle \right) \right\},
\end{aligned}$$

and

$$\begin{aligned}
\langle |x|^2 u_j, u_k \rangle &= \frac{A_j A_k}{L_j L_k} \left\langle \left(L_j^2 |y_j|^2 + 2L_j y_j \cdot X_j + |X_j|^2 \right) b_{j,1}, b_{k,1} \right\rangle \\
&= \frac{A_j A_k}{L_j L_k} \left\{ L_j^2 \langle b_{j,4}, b_{k,1} \rangle + 2L_j X_j \cdot \begin{pmatrix} \langle b_{j,2}, b_{k,1} \rangle \\ \langle b_{j,3}, b_{k,1} \rangle \end{pmatrix} + |X_j|^2 \langle b_{j,1}, b_{k,1} \rangle \right\}.
\end{aligned}$$

We also have

$$E_{0,1} = \langle u|u|^2, u \rangle = \sum_{j=1}^{N} \frac{A_j}{L_j} \langle u|u|^2, b_{j,1} \rangle.$$

We now proceed to computing the momentum, given by

$$M_{\mu,\lambda} = \left(E_{\mu,\lambda} - \mu \|xu\|_{\mathbb{L}^2}^2 \right)^2 + \mu^2 \left(\Im \int x \cdot \nabla u \bar{u} \right)^2.$$

We know how to compute $E_{\mu,\lambda}$ from previously, as well as $\|xu\|_{\mathbb{L}^2}^2 = \langle |x|^2 u, u\rangle$. It only remains to compute

$$\begin{aligned}\int x \cdot \nabla u \bar{u} &= \sum_{j,k=1}^{N} \frac{A_j A_k}{L_j L_k} \left\langle (L_j y_j + X_j) \cdot \left(i\beta_j - \frac{2+iB_j}{2L_j} y_j \right) b_{j,1}, b_{k,1} \right\rangle \\ &= \sum_{j,k=1}^{N} \frac{A_j A_k}{L_j L_k} \left\{ iL_j\beta_j \cdot \begin{pmatrix} \langle b_{j,2}, b_{k,1}\rangle \\ \langle b_{j,3}, b_{k,1}\rangle \end{pmatrix} - \frac{2+iB_j}{2} \langle b_{j,4}, b_{k,1}\rangle \right. \\ &\qquad \left. + i\beta_j \cdot X_j \langle b_{j,1}, b_{k,1}\rangle - \frac{2+iB_j}{2L_j} X_j \cdot \begin{pmatrix} \langle b_{j,2}, b_{k,1}\rangle \\ \langle b_{j,3}, b_{k,1}\rangle \end{pmatrix} \right\}.\end{aligned}$$

Note that all the inner products involved have already been computed when creating the DFMP matrix.

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