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On a Bubble algorithm for the cubic Nonlinear Schrödinger equation

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Abstract

Based on very recent and promising ideas, stemming from the use of *bubbles*, we discuss an algorithm for the numerical simulation of the cubic nonlinear Schrödinger equation with harmonic potential (cNLS) in any dimension, that could easily be extended to other polynomial nonlinearities. This algorithm consists in discretizing the initial function as a sum of modulated complex gaussian functions (the bubbles), each one having its own set of parameters, and then updating the parameters according to cNLS. Numerically, we solve exactly the linear part of the equation and use the Dirac-Frenkel-MacLachlan principle to approximate the nonlinear part. We then obtain a grid free algorithm in any dimension whose efficiency compared with spectral methods is illustrated by 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,

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

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 : $\Delta_x = \sum_{i=1}^d \partial_{x_i}^2$. This equation is also sometimes called *time-dependent Gross-Pitaevskii equation* [CCP⁺00, BJM03, Wan17, TTK22]. We focus on a cubic non-linearity 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*. The Schrödinger equation (cNLS) can be split into two parts, namely the linear and nonlinear parts:

$$i\partial_t\psi + \Delta_x\psi - |x|^2\psi = 0, \quad (\text{HO})$$

and

$$i\partial_t\psi = \psi|\psi|^2. \quad (\text{cNLS-nonLin.})$$

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 part,

like Lie, Strang Splitting or triple jump composition, see for instance [MQ02, HLW06, CCFM17]. However, the discretization of each of these two parts remain to be done using time and space discretization.

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

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

where

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

and $N \in \mathbb{N}^*$. We shall call each modulated function u_j a *bubble*.

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 was formerly called *Variational Gaussian wave packets* by Lasser and Lubich [LL20], where they applied the Dirac-Frenkel-MacLachlan principle (DFMP) to (HO). The Dirac-Frenkel-MacLachlan is the name given to the Dirac-Frenkel principle, or the MacLachlan principle, because in this case they are equivalent.

This method 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 (HO), the difference lying in the way the parameters are updated and how. For example, the Thawed Gaussian method allows the width matrix to be time-dependent while the Frozen Gaussian does not. However, they all produce an approximate solution, even in the linear case. In general, the chemists' setting of Gaussian beams involve correlated components, hence the width matrix. In the present paper we make the simplifying assumption that our gaussians are not correlated, and that their width is parametrized by a real positive scalar.

Let us explain the main ideas underlying the full modulation (1.2), and developed in various works, see for instance [MR18, FR20] and the references therein.

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 depending on the time through the parameters $(A, L, B, X, \beta, \gamma)$ and their time derivatives with respect to s , see (2.6) for more precise detail. It is then possible to choose the parameters in such a way that

$P(s; y, \partial_y)v = -\lambda v$ for some $\lambda \in \mathbb{R}$, and to take v as a soliton solution of the stationary equation

$$-\Delta_y v + |y|^2 v + |v|^2 v = \lambda v. \quad (1.3)$$

This yields to a differential system to be solved by the parameters $(A, L, B, X, \beta, \gamma)$ which is given below by the equations (2.7). It turns 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*.

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 several modulated solitons $N \geq 2$ are in interactions, this can produce finite time blow-up of growth of Sobolev norm phenomena, and 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 Szegő equation [GLPR18].

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

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

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 applied to the latter equation but we will restrict our analysis to the Harmonic case). Let us also note that such modulation technics 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 approximate solutions to the equations (HO) and (cNLS) by modulating the parameters $A_j, L_j, B_j, X_j, \beta_j, \gamma_j$ in such a way that $v_j(s_j, x)$ satisfies a *smoother in time* equation - typically a stationary soliton equation. From the numerical point of view, however, 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 on 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 part which would typically destroy the soliton structure in the equation.

This is why we decide here to use Gaussians for the functions v_j . Let us remark that in the case of small nonlinearities, ground states solitons are close to gaussians which makes the approximation relevant.

This Gaussian choice has the main following advantages : First we can solve exactly the linear part by using the classical modulation equations. Second, we can calculate explicitly the nonlinear interactions obtained by applying the Dirac-Frenkel-MacLachlan principle on the manifold of modulated gaussians to polynomial interactions. In the end, we thus obtain an algorithm for modulated Gaussians that can be easily implemented numerically, grid free, and able to capture high oscillations of the solution.

The paper is organized as follows. Section 2 is devoted to (HO) and can be seen as a specialization of [LL20] for a quadratic potential. We recall some conservation laws

and growth estimates when considering *bubbles* in (cNLS), as well as exhibit *modulation equations* which turn to have a completely integrable Hamiltonian structure. Those equations allow us to obtain an analytical formula for most of the modulation parameters. By choosing a shape for those bubbles – in our case gaussian – all of the modulation parameters can be obtained exactly.

The second part of this work takes into account cubic interactions, which were not accounted for in [LL20]. We focus in Section 3 on (cNLS-nonLin.). 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. This allows us to take into account as many bubbles as one desires at the cost of a computational complexity of order $\mathcal{O}(N^4d + d^3N^3)$. Here, N is the total number of bubbles. The fourth power of N is due to polynomial interactions of order three. This complexity almost does not suffer from the well-known “curse of dimensionality” since it is at most polynomial with respect to the dimension d . This relies on the exact computations of all of the integrals involved, hence we do not need to use numerical integration.

Finally, Section 4 is dedicated to illustrating numerically the fine details that are obtainable with the Dirac-Frenkel-MacLachlan principle (abbreviated DFMP), 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 DFMP 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 General case: $v = v(s, y)$

2.1.1 Conservation Laws

We recall classical laws for the Harmonic oscillator equation (see for instance [KV13, Tao06]). Let ψ be the solution to (HO). We will need the following result, known as the Pohozaev identity.

Lemma 2.1 (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*

$$\int \Delta f \left(\frac{d}{2} f + x \cdot \nabla f \right) dx = - \int |\nabla f|^2 dx. \quad (2.1)$$

Proof. By density, we only need to prove equation (2.1) 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

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

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

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

We integrate by parts the LHS, and obtain (2.1). \square

Lemma 2.2 (Conserved quantities in dimension $d = 2$). *The (radial) conservation laws are mass $\|u\|_{\mathbb{L}^2}$, energy*

$$E_0 = \frac{1}{2} \langle H\psi, \psi \rangle, \quad \text{where } H = -\Delta + |x|^2,$$

and momentum

$$M_0 = -2E_0 \|x\psi\|_{\mathbb{L}^2}^2 + \|x\psi\|_{\mathbb{L}^2}^4 + \left(\Im \int x \cdot \nabla \psi(x) \bar{\psi}(x) dx \right)^2,$$

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

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

Proof. For the momentum, we compute

$$\frac{1}{2} \frac{d}{dt} \int |x|^2 |\psi|^2 = 2 \Im \int x \cdot \nabla \psi \bar{\psi},$$

and

$$\frac{1}{2} \frac{d}{dt} \Im \int x \cdot \nabla \psi \bar{\psi} = \int |\nabla \psi|^2 - \int |x|^2 |\psi|^2 + \Re \left(\int x \cdot \nabla \psi \Delta \bar{\psi} \right).$$

We then use the Pohozaev identity (2.1), which yields

$$\frac{1}{2} \frac{d}{dt} \Im \int x \cdot \nabla \psi \bar{\psi} = \int |\nabla \psi|^2 - \int |x|^2 |\psi|^2 = 2E_0 - 2 \int |x|^2 |\psi|^2.$$

From this we obtain

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

Hence, the conservation laws

$$\begin{aligned} & \frac{1}{16} \left(\frac{d}{dt} \left[\Im \int x \cdot \nabla \psi \bar{\psi} \right] \right)^2 + \left(\Im \int x \cdot \nabla \psi \bar{\psi} \right)^2 \\ &= \left(E_0 - \|x\psi\|_{\mathbb{L}^2}^2 \right)^2 + \left(\Im \int x \cdot \nabla \psi \bar{\psi} \right)^2 \\ &= E_0^2 - 2E_0 \|x\psi\|_{\mathbb{L}^2}^2 + \|x\psi\|_{\mathbb{L}^2}^4 + \left(\Im \int x \cdot \nabla \psi \bar{\psi} \right)^2. \end{aligned}$$

Then

$$\frac{d}{dt} \Im \int \partial_j \psi \bar{\psi} = -2 \Im \int \partial_t \psi \bar{\partial}_j \bar{\psi} = 2 \Re \int i \partial_t \psi \bar{\partial}_j \bar{\psi} = 2 \Re \int |x|^2 \psi \bar{\partial}_j \bar{\psi} = -2 \int x_j |\psi|^2,$$

and

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

Hence the relations

$$\begin{cases} \frac{d}{dt} \int x_j |\psi|^2 = 2 \Im \int \partial_j \psi \bar{\psi} \\ \frac{d}{dt} \Im \int \partial_j \psi \bar{\psi} = -2 \int x_j |\psi|^2, \end{cases}$$

which have the conservation law

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

□

2.1.2 Renormalized flow

Recall the expression (1.2) of a bubble:

$$u(t, x) = \frac{A}{L} e^{i\gamma + iL\beta \cdot y - i\frac{B}{4}|y|^2} v(s, y), \quad y = \frac{x - X(t)}{L(t)}, \quad \frac{ds}{dt} = \frac{1}{L(t)}. \quad (2.2)$$

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

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

and

$$\partial_k \left[e^{iL\beta \cdot y - i\frac{B}{4}|y|^2} v \right] = e^{iL\beta \cdot y - i\frac{B}{4}|y|^2} \left[\partial_k v + i \left(L\beta_k - \frac{B}{2} y_k \right) v \right], \quad k = 1, \dots, d, \quad (2.3)$$

and

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

Hence,

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

We have

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

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

thus

$$\begin{aligned} -Hu &= \frac{A}{L^3} e^{i\gamma + iL\beta \cdot y - i\frac{B}{4}|y|^2} \left\{ \Delta_y v - iB \left(\frac{d}{2} v + \Lambda v \right) - L^2 (|\beta|^2 + |X|^2) v \right. \\ &\quad \left. + 2iL\beta \cdot \nabla v + (LB\beta - 2L^3 X) \cdot yv + \left(-\frac{B^2}{4} - L^4 \right) |y|^2 v \right\}, \end{aligned} \quad (2.4)$$

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

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

and hence

$$\begin{aligned} i\partial_t u &= e^{i\gamma + i\beta \cdot (x-X) - i\frac{B}{4L^2}|x-X|^2} \frac{A}{L^3} \left\{ i\partial_s v + (-\gamma_s + \beta \cdot X_s) v + \left(\frac{A_s}{A} - \frac{L_s}{L} \right) i v - \frac{L_s}{L} i \Lambda v \right. \\ &\quad \left. - i \frac{X_s}{L} \cdot \nabla v + \left(-L\beta_s - \frac{B X_s}{2L} \right) \cdot yv + \left(\frac{B_s}{4} - \frac{B L_s}{2L} \right) |y|^2 v \right\}. \end{aligned} \quad (2.5)$$

This yields

$$\begin{aligned} i\partial_t u - Hu &= \frac{A}{L^3} e^{i\gamma + iL\beta \cdot y - i\frac{B}{4}|y|^2} \left\{ i\partial_s v + \left(-\gamma_s + \beta \cdot X_s - L^2 (|\beta|^2 + |X|^2) \right) v \right. \\ &\quad + \left(\frac{A_s}{A} - \frac{L_s}{L} - B \frac{d}{2} \right) i v + \left(-\frac{L_s}{L} - B \right) i \Lambda v + i \left(2L\beta - \frac{X_s}{L} \right) \cdot \nabla v \\ &\quad + \left(-2L^3 X + LB\beta - L\beta_s - \frac{B X_s}{2L} \right) \cdot yv \\ &\quad \left. + \Delta_y v + \left[\frac{B_s}{4} - \left(\frac{B^2}{4} + L^4 \right) - \frac{B L_s}{2L} \right] |y|^2 v \right\} (s, y). \end{aligned} \quad (2.6)$$

2.1.3 Hamiltonian formulation for the free bubble

The one free bubble corresponds to the modulation equations

$$\begin{cases} -\gamma_s + \beta \cdot X_s - L^2(|\beta|^2 + |X|^2) = 0 \\ \frac{A_s}{A} - \frac{L_s}{L} - \frac{B}{2}d = 0 \\ -\frac{L_s}{L} - B = 0 \\ X_s = 2L^2\beta \\ -2L^3X + LB\beta - L\beta_s - \frac{BX_s}{2L} = 0 \\ \frac{B_s}{4} - \left(\frac{B^2}{4} + L^4\right) - \frac{B}{2}\frac{L_s}{L} = -1, \end{cases}$$

or equivalently

$$\begin{cases} A_s = \frac{AB}{2}(d-2) \\ L_s = -BL \\ B_s = -4 + 4L^4 - B^2 \\ X_s = 2L^2\beta \\ \beta_s = -2L^2X \\ \gamma_s = L^2(|\beta|^2 - |X|^2). \end{cases} \quad (2.7)$$

If the parameters are solutions to system (2.7), the function v then has to solve the Harmonic Oscillator with respect to time s and space y .

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

$$\begin{cases} A_t = \frac{AB}{2L^2}(d-2) \\ L_t = -\frac{B}{L} = -2L\partial_B\mathcal{E} \\ B_t = -\frac{4}{L^2} + 4L^2 - \frac{B^2}{L^2} = 2L\partial_L\mathcal{E} \\ X_t = 2\beta = \nabla_\beta\mathcal{R} \\ \beta_t = -2X = -\nabla_X\mathcal{R} \\ \gamma_t = |\beta|^2 - |X|^2, \end{cases} \quad (2.8)$$

with

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

Then we set

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

and the system becomes

$$\begin{cases} A_t = \frac{AB}{2}(d-2)e^{-4k} \\ k_t = -\partial_B \mathcal{H} \\ B_t = \partial_k \mathcal{H} \\ X_t = \nabla_\beta \mathcal{H} \\ \beta_t = -\nabla_X \mathcal{H} \\ \gamma_t = |\beta|^2 - |X|^2, \end{cases} \quad (2.9)$$

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 2.3. *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*

$$E(h, a, \xi, \theta) = 4h + 2|a|^2, \quad (2.10)$$

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

$$\begin{aligned} a(t) &= a(0), \\ \theta(t) &= \theta(0) + 2t, \\ h(t) &= h(0), \\ \xi(t) &= \xi(0) - 4t. \end{aligned} \quad (2.11)$$

We have the explicit formulae:

$$\begin{aligned} A(t) &= A(0) \left(\frac{L(t)}{L(0)} \right)^{\frac{2-d}{2}}, \\ e^{4k(t)} &= L(t)^2 = 2h(t) - \cos(\xi(t)) \sqrt{4h(t)^2 - 1}, \\ B(t) &= 2 \sin(\xi(t)) \sqrt{4h(t)^2 - 1}, \\ X_i(t) &= \sin(\theta_i(t)) \sqrt{2a_i(t)}, \quad i = 1, \dots, d, \\ \beta_i(t) &= \cos(\theta_i(t)) \sqrt{2a_i(t)}, \quad i = 1, \dots, d, \\ \gamma(t) &= \gamma(0) + \sum_{l=1}^d a_l(0) [\sin(2\theta_l(t)) - \sin(2\theta_l(0))] \end{aligned} \quad (2.12)$$

Proof. For the (X, β) part, it suffices to check that

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

are solutions. The expression for $\gamma(t)$ will be computed later within the proof of Lemma 2.5. 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:

$$B = 2\sqrt{e^{4k}\mathcal{E} - e^{8k} - 1}. \quad (2.13)$$

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 $-z^2 + \mathcal{E}z - 1$,

$$e^{4k_0} = \frac{1}{2} (\mathcal{E} - \sqrt{\mathcal{E}^2 - 4}), \quad e^{4k_1} = \frac{1}{2} (\mathcal{E} + \sqrt{\mathcal{E}^2 - 4}). \quad (2.14)$$

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

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

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 (2.14) 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 $\frac{dh}{dt} = 0$ and $\frac{d\xi}{dt} = -4$. Moreover,

$$\xi = \arcsin\left(\frac{e^{4k} - \frac{\mathcal{E}}{2}}{\sqrt{\frac{\mathcal{E}^2}{4} - 1}}\right) + \frac{\pi}{2} \in [0, \pi], \quad (2.15)$$

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 (2.13) 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 $\xi \in [0, \pi]$.

Finally, it remains to integrate the ODE on A , which 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

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

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

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

One can easily check that we have the following equality:

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

Note that, unless $h(0) = \frac{1}{2}$ or $h(t) = \frac{1}{2}$, these quantities are well-defined since $2h(s) > \sqrt{4h(s)^2 - 1}$, $s \in \{0, t\}$. 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 $L(t)^2$, hence the claimed result. \square

In practice, one would know the parameters $(A, L, B, X, \beta, \gamma)$ and would apply equation (2.12) in order to update them. We have the following result, which allows to obtain action-angle variables from the bubble's parameters:

Lemma 2.4. *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 $\theta(0)$ 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 $A(t)$, $L(t)$, $B(t)$, $X(t)$ and $\beta(t)$ will not depend on the value.

Note that to define $\xi(0)$ we could also use equation (2.15), but this is not appropriate from a computational point of view. Some more details are given in Remark 2.1.

Proof. We have $a_i(0) = \frac{1}{2} (X_i(0)^2 + \beta_i(0)^2)$, $i = 1, \dots, d$. 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

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

We also have

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

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,

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

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

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

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 rigorously 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 $A(t) = A(0) (L(t)/L(0))^{\frac{2-d}{2}}$. \square

2.2 A particular case: $v(s, y) = e^{-\frac{1}{2}|y|^2}$

When we have chosen the modulation equations (2.8), we chose them so that v is itself solution to the Harmonic Oscillator in time s and space y . This could maybe ease the process of finding a solution, but we can do even better: if we consider a particular expression for the function v we are also able to compute its time derivative and its laplacian in (2.6). By doing so, we can take into account those operators within new modulation equations.

We then have to choose a particular shape for the functions v . Note that the treatment of each bubble j is done separately, hence each function v_j can have its own shape different from the others. For simplicity, we take all the functions v_j to be gaussian functions. There are two main reasons for this choice: the first one is that when the width of a normalized gaussian function tend to zero, we can assimilate the function to a Dirac mass and hence view the proposed algorithm as an exact particle algorithm. The second reason is that we will have to consider the shapes of the functions v_j when we will add cubic interactions, and the gaussian functions allow us to perform most of the computations exactly, which greatly reduces the computational complexity and improves its accuracy. The gaussian shape is also motivated by the idea of Gaussian Beams.

From now on, the bubbles will have the following expression:

$$u_j(t, x) := \frac{A_j}{L_j} e^{i\gamma_j + iL_j\beta_j \cdot y_j - i\frac{B_j}{4}|y_j|^2} e^{-\frac{1}{2}|y_j|^2}, \quad \text{with} \quad y_j := \frac{x - X_j}{L_j}. \quad (2.17)$$

Since equation (HO) is linear with respect to ψ , if we use the ansatz (1.1) then we have to solve the Harmonic Oscillator equation for each bubble j :

$$i\partial_t u_j = -\Delta_x u_j + |x|^2 u_j \quad (2.18)$$

We can reuse equation (2.6) with $v_j(s_j, y_j) = e^{-\frac{|y_j|^2}{2}}$, and take advantage of the following equality:

$$\Delta_y v(y) = \Delta_y \left(e^{-\frac{|y|^2}{2}} \right) = (|y|^2 - d) v$$

This yields almost the same system of equations as (2.7): only the equation on γ_s changes, and we have

$$(\gamma_j)_s = L^2 (|\beta|^2 - |X|^2) - d.$$

With respect to time t , we get

$$(\gamma_j)_t = |\beta|^2 - |X|^2 - \frac{d}{L^2}. \quad (2.19)$$

If the parameters satisfy the modulation equations (2.8) (where the equation on γ_t has been changed to (2.19)), we have

$$i\partial_t u_j - H u_j = 0,$$

i.e. the Harmonic oscillator equation is automatically satisfied for the bubble j . Furthermore, we have the following result:

Lemma 2.5. Equation (2.19) can be integrated explicitly by using equation (2.12), and we have

$$\begin{aligned} \gamma(T) = \gamma(0) &+ \sum_{l=1}^d a_l(0) [\sin(2\theta_l(T)) - \sin(2\theta_l(0))] \\ &+ \frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} - 2T \right) \right) \\ &- \frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2}, \end{aligned} \quad (2.20)$$

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

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 mapping $t \mapsto \gamma(t)$.

Proof. We now proceed to the direct integration of γ_t .

$$\gamma(T) - \gamma(0) = \int_0^T \dot{\gamma}(t) dt = \int_0^T \left[|\beta(t)|^2 - |X(t)|^2 - \frac{d}{L(t)^2} \right] dt.$$

We have

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

and owing to (2.12):

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

Recall the following trig. identity:

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

hence

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

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

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

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

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

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

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

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

$$\int_0^T \frac{d}{L(t)^2} dt$$

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

Hence

$$\begin{aligned}
-\int_0^T \frac{d}{L(t)^2} dt &= \frac{d}{2} \arctan \left((c_1 + c_2) \tan \left(\frac{\xi(0)}{2} - 2T \right) \right) \\
&\quad - \frac{d}{2} \arctan \left((c_1 + c_2) \tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2}.
\end{aligned}$$

Finally, it remains to show that if $a_i(0) = 0$, $i \in \{1, \dots, d\}$ or $h(0) = \frac{1}{2}$, then the behavior of $t \mapsto \gamma(t)$ does not depend on the exact value of $\theta_i(0)$, $i \in \{1, \dots, d\}$ or $\xi(0)$. The exact formula for $\gamma(T)$ is:

$$\begin{aligned}
\gamma(T) &= \gamma(0) + a_1(0) [\sin(2\theta_1(T)) - \sin(2\theta_1(0))] \\
&\quad + a_2(0) [\sin(2\theta_2(T)) - \sin(2\theta_2(0))] \\
&\quad + \frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} - 2T \right) \right) \\
&\quad - \frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2}.
\end{aligned}$$

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

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

so that

$$\begin{aligned}
&\frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} - 2T \right) \right) \\
&\quad - \frac{d}{2} \arctan \left(\left(2h(0) + \sqrt{4h(0)^2 - 1} \right) \tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2}
\end{aligned}$$

$$= \frac{d}{2} \arctan \left(\tan \left(\frac{\xi(T)}{2} \right) \right) - \arctan \left(\tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2}$$

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

$$\begin{aligned} & \frac{d}{2} \arctan \left(\tan \left(\frac{\xi(T)}{2} \right) \right) - \frac{d}{2} \arctan \left(\tan \left(\frac{\xi(0)}{2} \right) \right) - m_T \frac{\pi d}{2} \\ &= \frac{d}{2} \frac{\widetilde{\xi(T)}}{2} - \frac{d}{2} \frac{\widetilde{\xi(0)}}{2} - m_T \frac{\pi d}{2} \\ &= \frac{d}{2} \frac{\xi(T)}{2} - (m_0 - m_T) \frac{\pi d}{2} - \frac{d}{2} \left(\frac{\xi(0)}{2} - m_0 \pi \right) - m_T \frac{\pi d}{2} \\ &= \frac{d}{2} \left(\frac{\xi(T)}{2} - \frac{\xi(0)}{2} \right) = -Td. \end{aligned}$$

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 $\xi(0)$. \square

Using Lemmata 2.3 and 2.4, we are now able to obtain an easy numerical algorithm which simulates 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 $j = 1, \dots, N$ **do** $\triangleright j$ denotes a bubble's index
 Use (2.16) to get the action-angle variables (h, a, ξ, θ) at time 0.
 Use (2.11) to update the variables (h, a, ξ, θ) up to time T .
 Use (2.12) (with the expression for $\gamma(t)$ replaced by (2.20)) to get the parameters of bubble u_j at time T .
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 (2.15). 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 $t \mapsto (L(t), B(t), X(t), \beta(t), \gamma(t))$.
- 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. 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]. Let \mathcal{M} be a manifold of complex-valued Gaussian functions:

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

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,

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

Remark 3.1. 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

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

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

$$\begin{aligned} \partial_t u(t) &\in \mathcal{T}_{u(t)}\mathcal{M}, \quad \text{such that} \\ \langle f, i\partial_t u(t) \rangle &= \langle f, u(t)|u(t)|^2 \rangle = 0, \quad \forall f \in B_{u(t)}. \end{aligned} \quad (3.3)$$

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

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

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

$$\langle i\partial_t u(t), b_{(d+2)(j-1)+l} \rangle = \langle u|u|^2, b_{(d+2)(j-1)+l} \rangle, \quad \forall j = 1, \dots, N, \quad l = 0, \dots, d+1. \quad (3.5)$$

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 to obtain ODEs on the parameters, and be able to integrate them 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, for which we know the value of the parameters.

In order to obtain the linear system, we first have to recall the expression of $i\partial_t u(t)$ (2.5):

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

More concisely, we have

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

where

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

and where $E_j^{(k)(1, \dots, d)}$ denotes the vector $(E_j^{(k)(1)}, \dots, E_j^{(k)(d)})$. 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:

$$\mathbf{A}\mathbf{E} = S, \tag{3.9}$$

where

$$\mathbf{A} := \begin{pmatrix} \langle b_1, b_1 \rangle & i\langle b_1, b_1 \rangle & \dots & \langle b_{(d+2)N}, b_1 \rangle & i\langle b_{(d+2)N}, b_1 \rangle \\ \vdots & \vdots & & \vdots & \vdots \\ \langle b_1, b_{(d+2)N} \rangle & i\langle b_1, b_{(d+2)N} \rangle & \dots & \langle b_{(d+2)N}, b_{(d+2)N} \rangle & i\langle b_{(d+2)N}, b_{(d+2)N} \rangle \end{pmatrix} \in \mathbb{C}^{(d+2)N, 2(d+2)N},$$

$$\mathbf{E} := \begin{pmatrix} \frac{A_1}{L_1^3} E_1^{(1)} \\ \frac{A_1}{L_1^3} E_1^{(2)} \\ \frac{A_1}{L_1^3} E_1^{(3)(1)} \\ \frac{A_1}{L_1^3} E_1^{(4)(1)} \\ \vdots \\ \frac{A_1}{L_1^3} E_1^{(3)(d)} \\ \frac{A_1}{L_1^3} E_1^{(4)(d)} \\ \frac{A_1}{L_1^3} E_1^{(5)} \\ \frac{A_1}{L_1^3} E_1^{(6)} \\ \vdots \\ \frac{A_N}{L_N^3} E_N^{(1)} \\ \frac{A_N}{L_N^3} E_N^{(2)} \\ \frac{A_N}{L_N^3} E_N^{(3)(1)} \\ \frac{A_N}{L_N^3} E_N^{(4)(1)} \\ \vdots \\ \frac{A_N}{L_N^3} E_N^{(3)(d)} \\ \frac{A_N}{L_N^3} E_N^{(4)(d)} \\ \frac{A_N}{L_N^3} E_N^{(5)} \\ \frac{A_N}{L_N^3} E_N^{(6)} \end{pmatrix} \in \mathbb{R}^{2(d+2)N}, \quad \text{and} \quad S := \begin{pmatrix} \langle u|u|^2, b_1 \rangle \\ \vdots \\ \langle u|u|^2, b_{(d+2)N} \rangle \end{pmatrix} \in \mathbb{C}^{(d+2)N}.$$

The matrix \mathbf{A} is the Gram matrix of the family $B_{u(t)}$ whose columns have been duplicated, which obviously depends on time. In order to solve the linear system (3.9) we shall

use the Moore-Penrose pseudo-inverse, which corresponds to the Least Squares solution if the matrix $\mathbf{A}^* \mathbf{A}$ is invertible. The pseudo-inverse 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.

Once the linear system (3.9) is solved, we obtain \mathbf{E} , from which we can update the modulation parameters. Using the definitions (3.8) we have, for $j = 1, \dots, N$,

$$\begin{aligned} \frac{A_j}{L_j^3} \begin{pmatrix} E_j^{(1)} \\ E_1^{(2)} \\ E_j^{(3)(1, \dots, d)} \\ E_j^{(4)(1, \dots, d)} \\ E_j^{(5)} \\ E_j^{(6)} \end{pmatrix} &= \mathfrak{R} \begin{pmatrix} \mathbf{E}_{2(d+2)j+1} \\ \vdots \\ \mathbf{E}_{2(d+2)(j+1)} \end{pmatrix} =: \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,1} \\ \vdots \\ \mathbf{E}_{j,2(d+2)} \end{pmatrix} \\ \iff \begin{pmatrix} \beta_j \cdot (X_j)_s - (\gamma_j)_s \\ \frac{(A_j)_s}{A_j} - \frac{(L_j)_s}{L_j} \\ -L_j(\beta_j)_s - \frac{B_j}{2L_j}(X_j)_s \\ \frac{(X_j)_s}{L_j} \\ \frac{(B_j)_s}{4} - \frac{B_j(L_j)_s}{2L_j} \\ \frac{(L_j)_s}{L_j} \end{pmatrix} &= \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,1} \\ \vdots \\ \mathbf{E}_{j,2(d+2)} \end{pmatrix}. \end{aligned}$$

Hence

$$\begin{aligned} \beta_j \cdot (X_j)_s - (\gamma_j)_s &= \mathfrak{R}(\mathbf{E}_{j,1}), \\ \frac{(A_j)_s}{A_j} - \frac{(L_j)_s}{L_j} &= \mathfrak{R}(\mathbf{E}_{j,2}), \\ -L_j(\beta_j)_s - \frac{B_j}{2L_j}(X_j)_s &= \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,3} \\ \vdots \\ \mathbf{E}_{j,d+2} \end{pmatrix}, \\ \frac{(X_j)_s}{L_j} &= \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,d+3} \\ \vdots \\ \mathbf{E}_{j,2d+2} \end{pmatrix}, \\ \frac{(B_j)_s}{4} - \frac{B_j(L_j)_s}{2L_j} &= \mathfrak{R}(\mathbf{E}_{j,2d+3}), \\ \frac{(L_j)_s}{L_j} &= \mathfrak{R}(\mathbf{E}_{j,2d+4}). \end{aligned}$$

Therefore

$$\begin{aligned}
(A_j)_s &= A_j \mathfrak{R}(\mathbf{E}_{j,2}) + A_j \mathfrak{R}(\mathbf{E}_{j,2d+4}), \\
(L_j)_s &= L_j \mathfrak{R}(\mathbf{E}_{j,2d+4}), \\
(B_j)_s &= 4\mathfrak{R}(\mathbf{E}_{j,2d+4}) + 2B_j \mathfrak{R}(\mathbf{E}_{j,2d+4}), \\
(X_j)_s &= L_j \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,d+3} \\ \vdots \\ \mathbf{E}_{j,2d+2} \end{pmatrix}, \\
(\beta_j)_s &= -\frac{1}{L_j} \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,3} \\ \vdots \\ \mathbf{E}_{j,d+2} \end{pmatrix} - \frac{B_j}{2L_j} \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,d+3} \\ \vdots \\ \mathbf{E}_{j,2d+2} \end{pmatrix}, \\
(\gamma_j)_s &= L_j \beta_j \cdot \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,3} \\ \vdots \\ \mathbf{E}_{j,d+2} \end{pmatrix} - \mathfrak{R}(\mathbf{E}_{j,1}),
\end{aligned}$$

and with respect to time t ,

$$\begin{aligned}
(A_j)_s &= \frac{A_j}{L_j^2} (\mathfrak{R}(\mathbf{E}_{j,2}) + \mathfrak{R}(\mathbf{E}_{j,2d+4})), \\
(L_j)_s &= \frac{1}{L_j} \mathfrak{R}(\mathbf{E}_{j,2d+4}), \\
(B_j)_s &= \frac{4}{L_j^2} \mathfrak{R}(\mathbf{E}_{j,2d+4}) + \frac{2B_j}{L_j^2} \mathfrak{R}(\mathbf{E}_{j,2d+4}), \\
(X_j)_s &= \frac{1}{L_j} \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,d+3} \\ \vdots \\ \mathbf{E}_{j,2d+2} \end{pmatrix}, \\
(\beta_j)_s &= -\frac{1}{L_j^3} \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,3} \\ \vdots \\ \mathbf{E}_{j,d+2} \end{pmatrix} - \frac{B_j}{2L_j^3} \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,d+3} \\ \vdots \\ \mathbf{E}_{j,2d+2} \end{pmatrix}, \\
(\gamma_j)_s &= \frac{1}{L_j} \beta_j \cdot \mathfrak{R} \begin{pmatrix} \mathbf{E}_{j,3} \\ \vdots \\ \mathbf{E}_{j,d+2} \end{pmatrix} - \frac{1}{L_j^2} \mathfrak{R}(\mathbf{E}_{j,1}).
\end{aligned} \tag{3.10}$$

3.1 Computing coefficients of the linear system (3.9)

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

$$\left\{ \begin{array}{l} z := \frac{2 + iB_l}{4L_l^2} + \frac{2 - iB_j}{4L_j^2}, \\ a := \frac{X_l}{L_l^2} + \frac{X_j}{L_j^2}, \\ \xi := \frac{B_j}{2L_j^2} X_j + \beta_j - \frac{B_l}{2L_l^2} X_l - \beta_l, \\ C = \exp \left\{ i(\gamma_l - \gamma_j) - \frac{2 + iB_l}{4L_l^2} |X_l|^2 - \frac{2 - iB_j}{4L_j^2} |X_j|^2 - i\beta_l \cdot X_l + i\beta_j \cdot X_j \right\}. \end{array} \right. \quad (3.11)$$

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 $n, m = 1, \dots, d$,

$$\begin{aligned} \langle b_{(d+2)(l-1)+1}, b_{(d+2)(j-1)+1} \rangle &= C \widehat{f}(\xi) \\ \langle b_{(d+2)(l-1)+n+1}, b_{(d+2)(j-1)+1} \rangle &= \frac{C}{L_l} \left(\widehat{x}f_n - (X_l)_n \widehat{f} \right) (\xi) \\ \langle b_{(d+2)l}, b_{(d+2)(j-1)+1} \rangle &= \frac{C}{L_l^2} \left(\widehat{|x|^2 f} - 2X_l \cdot \widehat{x}f + |X_l|^2 \widehat{f} \right) (\xi) \\ \langle b_{(d+2)(l-1)+n+1}, b_{(d+2)(j-1)+m+1} \rangle &= \frac{C}{L_j L_l} \left[\widehat{x_n x_m f} - (X_l)_n \widehat{x_m f} - (X_j)_m \widehat{x_n f} + (X_l)_n (X_j)_m \widehat{f} \right] (\xi) \\ \langle b_{(d+2)l}, b_{(d+2)(j-1)+m+1} \rangle &= \frac{C}{L_l^2 L_j} \left[\widehat{x_m |x|^2 f} - 2X_l \cdot \widehat{x_m x f} + |X_l|^2 \widehat{x_m f} \right. \\ &\quad \left. - (X_j)_m \widehat{|x|^2 f} + 2(X_j)_m X_l \cdot \widehat{x}f - |X_l|^2 (X_j)_m \widehat{f} \right] (\xi) \\ \langle b_{(d+2)l}, b_{(d+2)j} \rangle &= \frac{C}{L_l^2 L_j^2} \left[\widehat{|x|^4 f} - 2X_l \cdot \widehat{|x|^2 x f} + |X_l|^2 \widehat{|x|^2 f} - 2X_j \cdot \widehat{x|x|^2 f} \right. \\ &\quad \left. + 4 \sum_{n,m=1}^d (X_l)_n (X_j)_m \widehat{x_n x_m f} - 2|X_l|^2 X_j \cdot \widehat{x}f \right. \\ &\quad \left. + \widehat{|x|^2 f} |X_j|^2 - 2|X_j|^2 X_l \cdot \widehat{x}f + |X_l|^2 |X_j|^2 \widehat{f} \right] (\xi) \end{aligned}$$

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

$$\begin{aligned}
C_{\Im} &:= \exp \{i(\gamma_k + \gamma_l - \gamma_m - \gamma_j)\} \\
&\quad \times \exp \{i(\beta_j \cdot X_j + \beta_m \cdot X_m - \beta_l \cdot X_l - \beta_k \cdot X_k)\} \\
&\quad \times \exp \left\{ -i \left(\frac{B_k}{4L_k^2} |X_k|^2 + \frac{B_l}{4L_l^2} |X_l|^2 - \frac{B_m}{4L_m^2} |X_m|^2 - \frac{B_j}{4L_j^2} |X_j|^2 \right) \right\}, \\
C_{\Re} &:= \exp \left\{ -\frac{1}{2} \left(\frac{|X_k|^2}{L_k^2} + \frac{|X_l|^2}{L_l^2} + \frac{|X_m|^2}{L_m^2} + \frac{|X_j|^2}{L_j^2} \right) \right\}, \\
C &:= \frac{A_k A_l A_m}{L_k L_l L_m} C_{\Im} C_{\Re}, \\
\xi &:= - \left[\beta_k + \beta_l - \beta_m - \beta_j + \frac{B_k}{2L_k^2} X_k + \frac{B_l}{2L_l^2} X_l - \frac{B_m}{2L_m^2} X_m - \frac{B_j}{2L_j^2} X_j \right], \\
z &:= \frac{1}{2} \left(\frac{1}{L_k^2} + \frac{1}{L_l^2} + \frac{1}{L_m^2} + \frac{1}{L_j^2} \right) + i \left(\frac{B_k}{4L_k^2} + \frac{B_l}{4L_l^2} - \frac{B_m}{4L_m^2} - \frac{B_j}{4L_j^2} \right), \\
a &:= \frac{1}{L_k^2} X_k + \frac{1}{L_l^2} X_l + \frac{1}{L_m^2} X_m + \frac{1}{L_j^2} X_j.
\end{aligned} \tag{3.12}$$

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 $1 \leq r \leq d$,

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

We refer to Appendix A for more details. Moreover, Appendix B contains Table 1 which sums up the useful Fourier transforms.

Remark 3.2 (Computational complexity). In (2.17) we chose $v_j(s_j, y_j) = e^{-\frac{1}{2}|y_j|^2}$. This choice was made so that the inner products involved in the application of the DFMP are computable exactly. 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 $\mathcal{O}(N^4 d + N^2(d+2)^2)$. To obtain the total complexity, we have to add the cost computing the pseudo-inverse of the hermitian matrix $\mathbf{A} \in \mathbb{C}^{(d+2)N, (d+2)N}$, which is $\mathcal{O}((d+2)^3 N^3)$. This yields the overall computational complexity: $\mathcal{O}(N^4 d + d^3 N^3)$.

We obtain Algorithm 2 which can be used to obtain an approximate solution to (cNLS) as a sum of bubbles, using the Strang splitting.

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.

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** $\triangleright j$ denotes a bubble's index
 Use Algorithm 1 to update the bubbles over a timestep of size $dt/2$.
 Compute the coefficients of the linear system (3.9).
 Solve the linear system (3.9) to obtain \mathbf{E} .
 Use (3.10) to update the parameters over a timestep of size dt .
 Use Algorithm 1 to update the bubbles over a timestep of size $dt/2$.
 end for
end for

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.

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

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,

$$\begin{aligned} \frac{d}{dt} H_{\text{interactions}}(t) &= \frac{1}{4} \frac{d}{dt} \langle u(t)^2, u(t)^2 \rangle \\ &= \frac{1}{4} \langle 2u(t) \partial_t u(t), u(t)^2 \rangle + \langle u(t)^2, 2u(t) \partial_t u(t) \rangle \\ &= \Re \langle u(t) \partial_t u(t), u(t)^2 \rangle \\ &= \Re \langle \partial_t u(t), u(t) |u(t)|^2 \rangle. \end{aligned}$$

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,

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

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

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

□

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 (2.6) over $j = 1, \dots, N$ 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

$$\begin{aligned} \sum_{j=1}^N c_{(d+2)(j-1)+1} b_{(d+2)(j-1)+1} + c_{(d+2)(j-1)+2} b_{(d+2)(j-1)+2} + \dots \\ + c_{(d+2)(j-1)+d+1} b_{(d+2)(j-1)+d+1} + c_{(d+2)j} b_{(d+2)j} = 0. \end{aligned} \quad (3.13)$$

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

$$c_k = 0, \quad k = 1, \dots, (d+2)N. \quad (3.14)$$

This yields exactly the system of equations (2.7), with the γ equation replaced by (2.19). In other words, the DFMP approach gives the same equations as those given in Section 2.2 when $B_{u(t)}$ is a linearly independent family. However, our approach as described in Section 2.2 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 (3.14) anymore, hence the DFMP approach fails. Our approach allows to circumvent this issue by naturally imposing conditions (3.14) in all cases.

3.4 Imposing conservation of \mathbb{L}^2 norm

Our numerical experiments have shown that the DFMP approach does not always yield a nice conservation of the \mathbb{L}^2 norm, even though it should be conserved. This section is dedicated to finding a way of imposing it explicitly.

By using (3.7), the conservation of the \mathbb{L}^2 norm writes

$$\begin{aligned} 0 &= \partial_t \int_{\mathbb{R}^2} |u(t, x)|^2 = 2\Re \langle \partial_t u, u \rangle \\ &= 2 \sum_{k=1}^N \frac{A_k}{L_k^3} \Re \left\langle -i \left\{ b_{(d+2)(k-1)+1} \left(E_k^{(1)} + iE_k^{(2)} \right) \right. \right. \\ &\quad \left. \left. + b_{(d+2)(k-1)+2} \left(E_k^{(3)(1)} + iE_k^{(4)(1)} \right) \right. \right. \\ &\quad \left. \left. \vdots \right. \right. \\ &\quad \left. \left. + b_{(d+2)(k-1)+d+1} \left(E_k^{(3)(d)} + iE_k^{(4)(d)} \right) \right. \right. \\ &\quad \left. \left. + b_{(d+2)k} \left(E_k^{(5)} + iE_k^{(6)} \right) \right\}, u \right\rangle. \end{aligned}$$

Under matrix form, this yields

$$0 = 2\Im \left[\left(\langle b_1, u \rangle, i \langle b_1, u \rangle, \dots, \langle b_{(d+2)N}, u \rangle, i \langle b_{(d+2)N}, u \rangle \right) \mathbf{E} \right].$$

Since $\mathbf{E} \in \mathbb{R}^{2(d+2)N}$, we obtain

$$\left(\Im \langle b_1, u \rangle, \Re \langle b_1, u \rangle, \dots, \Im \langle b_{(d+2)N}, u \rangle, \Re \langle b_{(d+2)N}, u \rangle \right) \mathbf{E} = 0.$$

In order to impose the conservation of the \mathbb{L}^2 norm, we have to add this line to the linear system (3.9). Moreover, this line has already been computed: indeed, we have

$$u = \sum_{j=1}^N \frac{A_j}{L_j} b_{(d+2)(j-1)+1},$$

hence

$$\langle b_k, u \rangle = \sum_{j=1}^N \frac{A_j}{L_j} \langle b_k, b_{(d+2)(j-1)+1} \rangle, \quad k = 1, \dots, (d+2)N.$$

The idea motivating the addition of this line to the linear system is the following: whenever the pseudo-inverse of the matrix \mathbf{A} is well-conditioned the conservation of \mathbb{L}^2 norm is automatically satisfied, so the new line doesn't change anything. When the pseudo-inverse is ill-conditioned, it may happen that the \mathbb{L}^2 norm isn't preserved anymore. Hence, at each time step we compute the solution to the initial system of size $(d+2)N \times 2(d+2)N$, and if the variation of the \mathbb{L}^2 norm of u is too high (e.g. larger than some numerical threshold) then we solve again the augmented linear system.

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:

$$e^{-it(-\Delta+|x|^2)} = e^{-\frac{i}{2} \tanh(t)|x|^2} e^{\frac{i}{2} \sinh(2t)\Delta_x} e^{-\frac{i}{2} \tanh(t)|x|^2}. \quad (4.1)$$

We can cite [JMS11] which also presents a spectral method based on the Fourier transform with time splitting, however our 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: $e^{\frac{i}{2} \sinh(2t)\Delta_x}$ is the propagator of the following equation:

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

By using a Fourier transform, we get

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

Hence,

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

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 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.

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

```

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

```

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

```

Discretize the initial data  $\eta$  on a Grid  $\subset \mathbb{R}^d$ .
for Each timestep of size  $\Delta t$  do
  Use Algorithm 3 with a stepsize  $\Delta t/2$ .
  for  $x \in \text{GRID}$  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

```

Of course, in practical 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 $[-8, 8] \times [-8, 8]$ 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.

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 bubble without too much overlaps 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].

4.3 Observables

In order to compare the bubbles scheme against the spectral method, we first compare them in absence of interactions, i.e. on the Harmonic Oscillator (HO). We already showed in Lemma 2.2 the conservation of some quantities, these will be the ones we use for the comparisons. 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 C. 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, the spectral scheme is supplied with the exact initial condition and not the bubbles discretization.

4.4 Results

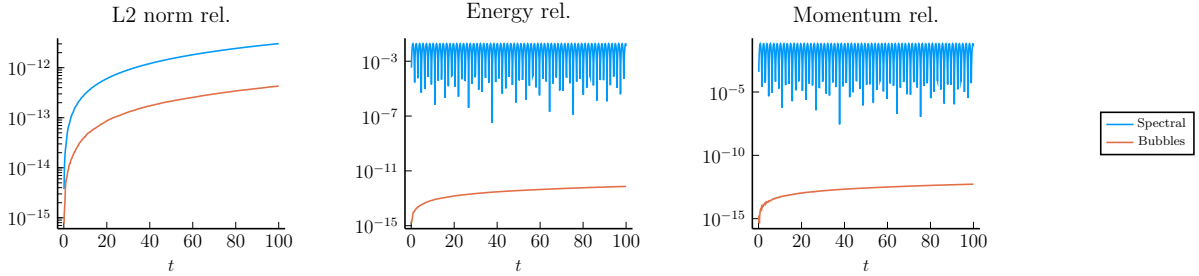
We consider examples adapted from [BJM03].

4.4.1 Test case 1: Zero phase initial data

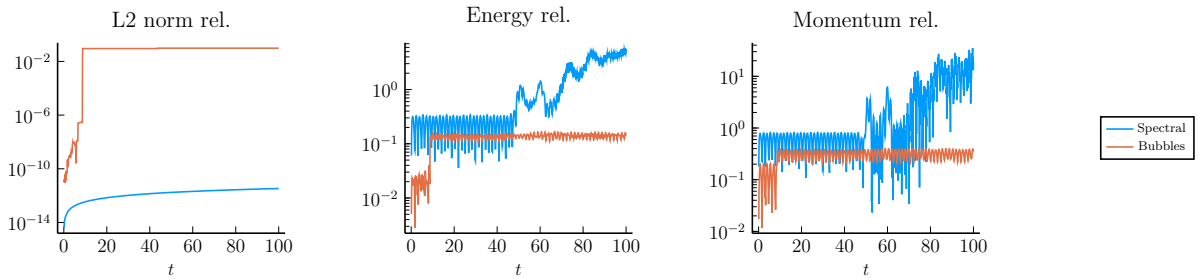
The initial condition reads

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

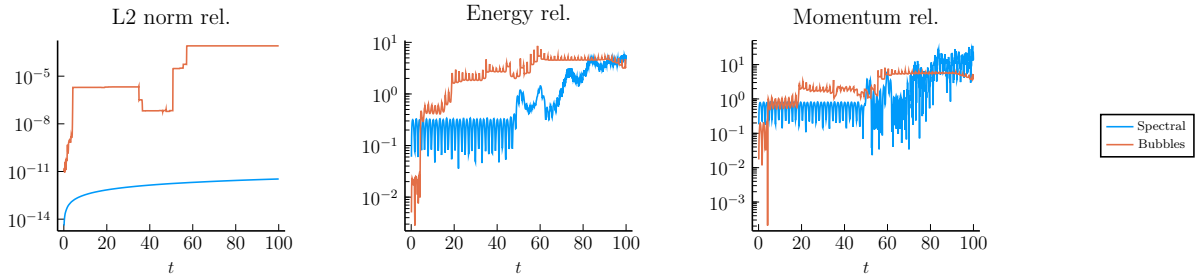
The results are displayed in Figure 1. The solution approximated with the DFMP outperforms the spectral method on both the Harmonic Oscillator and the cubic NonLinear Schrödinger equations. The conservative quantities are not exactly preserved in the latter equation, and exhibit some drift after some time. It is however about two orders of magnitude better for the DFMP approach when not imposing the conservation of the \mathbb{L}^2 norm. The ‘‘jumps’’ may be explained by an ill-conditioned Gram matrix, which would then yield a very rough approximation of the modulation parameters.



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



(b) Approximate solution to the Schrödinger equation (cNLS). DFMP approach with no enforcement of \mathbb{L}^2 norm.



(c) Approximate solution to the Schrödinger equation (cNLS). DFMP approach by imposing the conservation of the \mathbb{L}^2 norm.

Figure 1: Test case 1. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 5 \cdot 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 128$. Numerical tolerance on the variation of \mathbb{L}^2 norm: 10^{-8} .

We can note that if we impose the conservation of the \mathbb{L}^2 norm there are two phenomena occurring: the \mathbb{L}^2 norm is not preserved exactly even though we impose it, and the other conservative quantities exhibit a worse conservation. The first one can be explained by the fact that we only solve the linear system (3.9) with the Moore-Penrose pseudo-inverse, which amounts to solving least squares as long as bubbles do not overlap. Moreover, the least squares solution cannot yield a zero error since we are projecting on a low dimensional manifold and we lose information in this process: this is precisely what allows us to keep a solution which can be expressed as a sum of modulated gaussian functions. This means that the \mathbb{L}^2 norm cannot be exactly preserved even though we imposed it. We can however note that its conservation is better once that constraint is added into the linear system. The second phenomenon can be explained by the fact that the linear system obtained when imposing the conservation of the \mathbb{L}^2 norm is overdetermined.

4.4.2 Test case 2: Weak interactions

The initial condition reads

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

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.

In this example, the variation of the \mathbb{L}^2 norm is smaller than the numerical threshold we chose, hence the solution obtained when imposing the conservation of the \mathbb{L}^2 norm is the same solution as when it is not imposed.

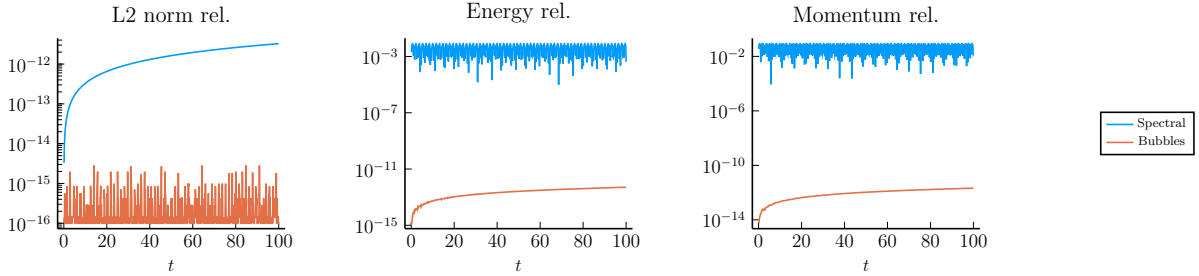
4.4.3 Test case 3: Strong interactions

The initial condition reads

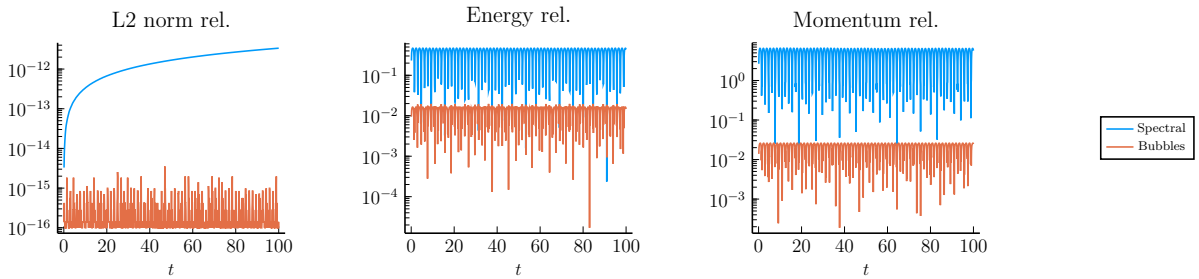
$$\psi(t = 0, x) = \begin{cases} \sqrt{M^2 - |x|^2} e^{i \cosh \sqrt{x_1^2 + x_2^2}}, & |x|^2 < M^2 \\ 0 & \text{otherwise} \end{cases}, \quad M = 4. \quad (4.4)$$

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 is 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.

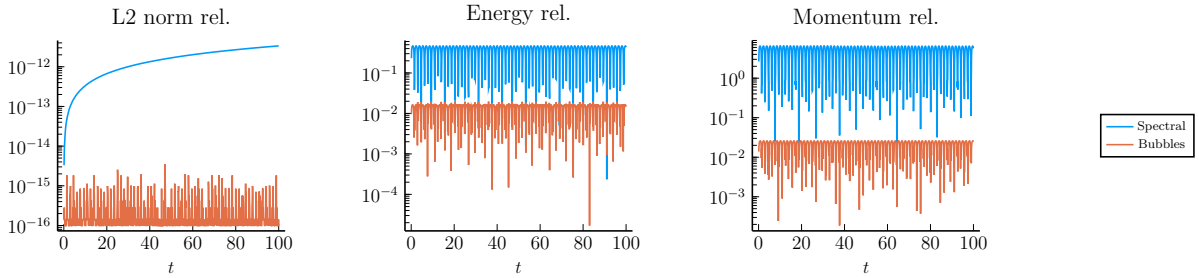
The results are displayed in Figure 4. This example is by far the most interesting of the three test cases presented in this paper, because it shows that with the discretization given in Figure 3 the conservation properties are pretty good with DFMP even when there are a lot of interactions between bubbles. Once again, the “jumps” in the relative evolution



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



(b) Approximate solution to the Schrödinger equation (cNLS). DFMP approach with no enforcement of \mathbb{L}^2 norm.



(c) Approximate solution to the Schrödinger equation (cNLS). DFMP approach by imposing the conservation of the \mathbb{L}^2 norm.

Figure 2: Test case 2. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 5 \cdot 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 128$. Numerical tolerance on the variation of \mathbb{L}^2 norm: 10^{-8} .

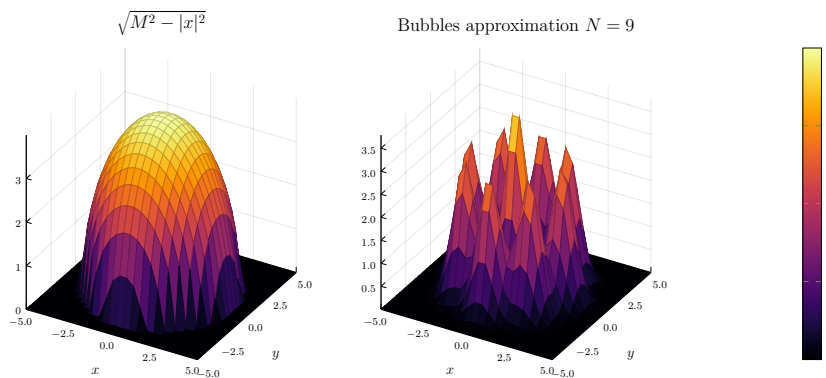


Figure 3: Approximation of $x \mapsto \sqrt{M^2 - |x|^2}$ as a sum of bubbles

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.

We can make here the same remarks about the solution obtained when imposing the conservation of the \mathbb{L}^2 norm as we made for test case 1.

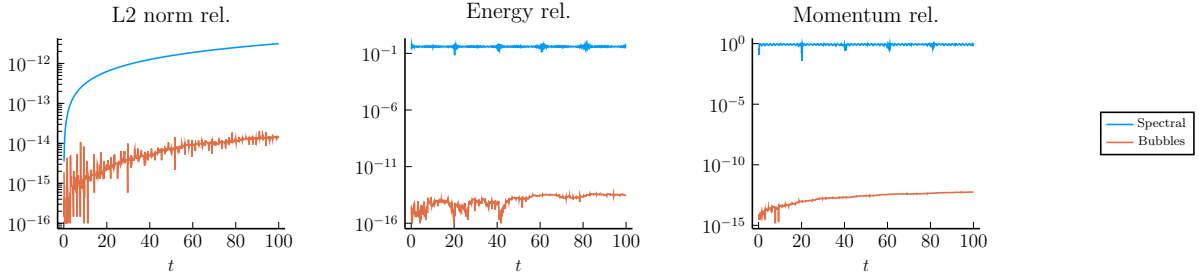
5 Conclusion

We presented in this work an approach based on recent results [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.

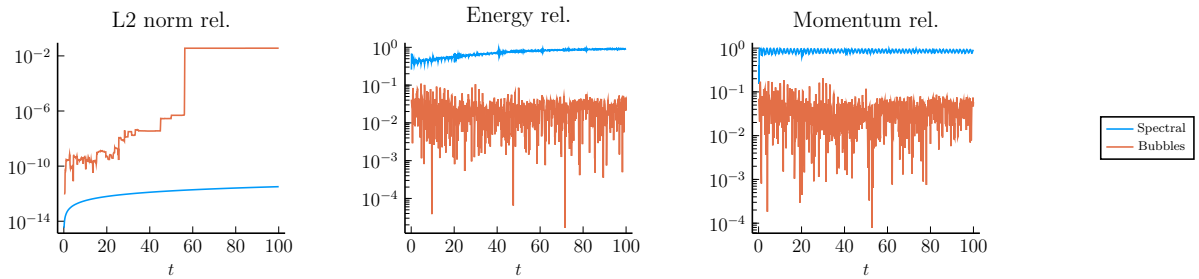
In this context we focused on a particular subclass of such functions, modulated gaussians, which have the advantage of allowing explicit computations. This is particularly interesting since we do not have to rely on any sort of discretization of the phase space, which is usually the main computational burden in numerical simulations. We obtain an algorithm which yields an exact solution as soon as the initial data is a sum of modulated gaussians. If we consider an arbitrary function, the only error this algorithm makes is the initial discretization of said function as a finite sum of modulated gaussians.

We also extended the results from [FR20] by allowing polynomial interactions, at the cost of approximating the solution to (cNLS-nonLin.) via the Dirac-Frenkel-MacLachlan principle. Once again, considering only modulated gaussian functions allowed us to perform explicit computations and to obtain a numerical algorithm whose computational complexity writes $\mathcal{O}(N^4d + N^3d^3)$. 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.

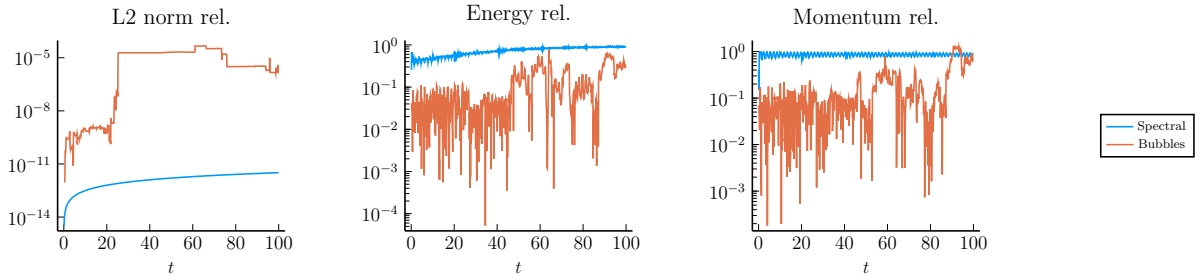
Finally, our numerical examples show that the bubbles algorithm outperforms a spectral method combined with time splitting, where each splitting step is solved exactly. We



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



(b) Approximate solution to the Schrödinger equation (cNLS). DFMP approach with no enforcement of \mathbb{L}^2 norm.



(c) Approximate solution to the Schrödinger equation (cNLS). DFMP approach by imposing the conservation of the \mathbb{L}^2 norm.

Figure 4: Test case 3. Relative evolution of mass, energy and momentum with bubbles and spectral methods. $\Delta t = 5 \cdot 10^{-3}$. Time-integrator for the nonlinear part of the splitting: Runge-Kutta of order 4. Spectral scheme with $N_x = 128, N_y = 128$. Numerical tolerance on the variation of \mathbb{L}^2 norm: 10^{-8} .

compared the results obtained when solving the Dirac-Frenkel-MacLachlan linear system, with and without imposing the conservation of the \mathbb{L}^2 norm: as expected, imposing the conservation of the \mathbb{L}^2 norm worsens the conservation of the energy and momentum.

As a final note, we emphasize the fact that 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.

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

A.1 Coefficients of the matrix A

$$\langle \underline{b_{(d+2)(l-1)+1}}, \underline{b_{(d+2)(j-1)+1}} \rangle.$$

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

Let

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

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

$$\langle b_{(d+2)l-d-1}, b_{(d+2)j-d-1} \rangle = C \int_{\mathbb{R}^d} e^{-i\xi \cdot x} f(x) dx = C \widehat{f}(\xi)$$

$$\langle \underline{b_{(d+2)(l-1)+n+1}, b_{(d+2)(j-1)+1}}, 1 \leq n \leq d. \rangle$$

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

$$\langle \underline{b_{(d+2)l}, b_{(d+2)(j-1)+1}} \rangle$$

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

$$\langle \underline{b_{(d+2)(l-1)+n+1}, b_{(d+2)(j-1)+m+1}}, 1 \leq n, m \leq d. \rangle$$

$$\begin{aligned} \langle b_{(d+2)(l-1)+n+1}, b_{(d+2)(j-1)+m+1} \rangle &= C \int_{\mathbb{R}^d} \frac{x_n - (X_l)_n}{L_l} \frac{x_m - (X_j)_m}{L_j} e^{-i\xi \cdot x} f(x) dx \\ &= \frac{C}{L_j L_l} \int_{\mathbb{R}^d} (x_n - (X_l)_n)(x_m - (X_j)_m) e^{-i\xi \cdot x} f(x) dx \\ &= \frac{C}{L_j L_l} \int_{\mathbb{R}^d} [x_n x_m - x_n (X_j)_m - x_m (X_l)_n + (X_l)_n (X_j)_m] \\ &\quad \times e^{-i\xi \cdot x} f(x) dx \\ &= \frac{C}{L_j L_l} [\widehat{x_n x_m f} - (X_l)_n \widehat{x_m f} - (X_j)_m \widehat{x_n f} + (X_l)_n (X_j)_m \widehat{f}] (\xi). \end{aligned}$$

$$\langle \underline{b_{(d+2)l}, b_{(d+2)(j-1)+m+1}}, 1 \leq m \leq d. \rangle$$

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

$$\langle \underline{b_{(d+2)l}, b_{(d+2)j}} \rangle$$

$$\langle b_{(d+2)l}, b_{(d+2)j} \rangle = C \int_{\mathbb{R}^d} e^{-i\xi \cdot x} e^{-z|x|^2 + a \cdot x} \frac{|x - X_l|^2}{L_l^2} \frac{|x - X_j|^2}{L_j^2} dx$$

$$\begin{aligned}
&= \frac{C}{L_l^2 L_j^2} \int_{\mathbb{R}^d} e^{-i\xi \cdot x} e^{-z|x|^2 + a \cdot x} \left(|x|^2 - 2x \cdot X_l + |X_l|^2 \right) \\
&\quad \times \left(|x|^2 - 2x \cdot X_j + |X_j|^2 \right) dx \\
&= \frac{C}{L_l^2 L_j^2} \int_{\mathbb{R}^d} e^{-i\xi \cdot x} e^{-z|x|^2 + a \cdot x} \left(|x|^4 - 2|x|^2 x \cdot X_l + |X_l|^2 |x|^2 \right. \\
&\quad \left. - 2(x \cdot X_j) |x|^2 + 4(x \cdot X_l)(x \cdot X_j) - 2(x \cdot X_j) |X_l|^2 \right. \\
&\quad \left. + |x|^2 |X_j|^2 - 2(x \cdot X_l) |X_j|^2 + |X_l|^2 |X_j|^2 \right) dx \\
&= \frac{C}{L_l^2 L_j^2} \left[\widehat{|x|^4 f} - 2X_l \cdot \widehat{|x|^2 x f} + |X_l|^2 \widehat{|x|^2 f} \right. \\
&\quad \left. - 2X_j \cdot \widehat{|x|^2 x f} + 4(x \cdot X_l)(x \cdot X_j) f - 2|X_l|^2 X_j \cdot \widehat{x f} \right. \\
&\quad \left. + \widehat{|x|^2 f} |X_j|^2 - 2|X_j|^2 X_l \cdot \widehat{x f} + |X_l|^2 |X_j|^2 \widehat{f} \right] (\xi)
\end{aligned}$$

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

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

A.2 Coefficients of the vector of interactions S

$\langle u|u|^2, b_{(d+2)(j-1)+1} \rangle$

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

We recall the previously defined notations:

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

Then,

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

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

and

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

Define

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

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

$$\langle u|u|^2, b_{(d+2)(j-1)+1} \rangle = \sum_{k,l,m} C \hat{f}(\xi). \quad (\text{A.2})$$

$$\underline{\langle u|u|^2, b_{(d+2)(j-1)+r+1} \rangle}, \quad r = 1, \dots, d$$

$$\langle u|u|^2, b_{(d+2)(j-1)+r+1} \rangle$$

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

$\langle u|u|^2, b_{(d+2)j} \rangle$

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

Appendix B Fourier transforms of Gaussians

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

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

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

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

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

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

\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:

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

Let

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

then

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

$h(x)$	$\widehat{h}(\xi)/e^{-\frac{(\xi+ia)\cdot(\xi+ia)}{4z}}$
f	$\left(\frac{\pi}{z}\right)^{\frac{d}{2}}$
xf	$-i\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\frac{\xi+ia}{2z}$
$x_mx_n f$	$-\frac{1}{4z^2}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}(\xi_n+ia_n)(\xi_m+ia_m)$
$x_m^2 f$	$\frac{1}{2z}\left(\frac{\pi}{z}\right)^{\frac{d}{2}}\left[1-\frac{(\xi_m+ia_m)^2}{2z}\right]$
$ 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 $f(x) = e^{-z|x|^2+ax}$, $z \in \mathbb{C}$, $\Re(z) > 0$, $a \in \mathbb{R}^d$.

and

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

Hence,

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

\widehat{xf} .

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

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

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

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

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

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

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

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

$$\widehat{x_m |x|^2 f}(\xi)$$

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

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

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

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

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

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

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

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

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

□

Appendix C Miscellaneous computations

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

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

We give the explicit expressions for the conservative quantities involved in Lemma 2.2, in the two-dimensional case.

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

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

The energy of a sum of bubbles is given by

$$\begin{aligned}
2E_0 &= \left\langle \sum_{j=1}^N H u_j(x), \sum_{k=1}^N u_k(x) \right\rangle \\
&= \sum_{j,k=1}^N \langle H u_j(x), u_k(x) \rangle \\
&= \sum_{j,k=1}^N \left(\langle \nabla_x u_j(x), \nabla_x u_k(x) \rangle + \langle |x|^2 u_j(x), u_k(x) \rangle \right)
\end{aligned}$$

We have

$$\begin{aligned}
\nabla_x u_k(x) &= \frac{A_k}{L_k} \frac{1}{L_k} \left[iL_k \beta_k - \frac{2 + iB_k}{2} \frac{x - X_k}{L_k} \right] e^{i\Gamma_k} e^{-\frac{1}{2} \left| \frac{x - X_k}{L_k} \right|^2} \\
&= \frac{A_k}{L_k} \left[i\beta_k - \frac{2 + iB_k}{2L_k^2} (x - X_k) \right] e^{i\Gamma_k} e^{-\frac{1}{2} \left| \frac{x - X_k}{L_k} \right|^2} \\
&= \frac{A_k}{L_k} \left[\underbrace{i\beta_k + \frac{2 + iB_k}{2L_k^2} X_k}_{=: \eta_k} - \frac{2 + iB_k}{2L_k^2} x \right] e^{i\Gamma_k} e^{-\frac{1}{2} \left| \frac{x - X_k}{L_k} \right|^2}
\end{aligned}$$

$$= \left[\underbrace{i\beta_k + \frac{2 + iB_k}{2L_k^2} X_k}_{=: \eta_k} - \frac{2 + iB_k}{2L_k^2} x \right] u_k(x),$$

and thus

$$\begin{aligned} |\nabla_x u(x)|^2 &= \nabla_x u(x) \cdot \overline{\nabla_x u(x)} \\ &= \sum_{k,l=1}^N \left[\eta_k - \frac{2 + iB_k}{2L_k^2} x \right] \cdot \left[\bar{\eta}_l - \frac{2 - iB_l}{2L_l^2} x \right] u_k(x) \bar{u}_l(x) \\ &= \sum_{k,l=1}^N \left[\eta_k \cdot \bar{\eta}_l - \frac{2 + iB_k}{2L_k^2} x \cdot \bar{\eta}_l - \frac{2 - iB_l}{2L_l^2} x \cdot \eta_k + \frac{2 - iB_l}{2L_l^2} \frac{2 + iB_k}{2L_k^2} |x|^2 \right] u_k(x) \bar{u}_l(x) \\ &= \sum_{k,l=1}^N \left[\eta_k \cdot \bar{\eta}_l - \left(\frac{2 + iB_k}{2L_k^2} \bar{\eta}_l + \frac{2 - iB_l}{2L_l^2} \eta_k \right) \cdot x + \frac{2 - iB_l}{2L_l^2} \frac{2 + iB_k}{2L_k^2} |x|^2 \right] u_k(x) \bar{u}_l(x) \end{aligned}$$

Finally, to obtain $\langle \nabla_x u(x), \nabla_x u(x) \rangle$ it suffices to integrate $|\nabla_x u(x)|^2$ over \mathbb{R}^d . We then recognize integrals that have already been computed in Appendix B.

We now proceed to computing the momentum, given by

$$M_0 = -2E_0 \|x\psi\|_{\mathbb{L}^2}^2 + \|xu\|_{\mathbb{L}^2}^4 + \left(\Im \int x \cdot \nabla u(x) \bar{u}(x) dx \right)^2.$$

We know how to compute E_0 from the previous computations. The norm $\|x\psi\|_{\mathbb{L}^2}^2$ has also already been computed in Appendix B. Thus, it only remains to compute the integral

$$\begin{aligned} \int x \cdot \nabla u(x) \bar{u}(x) dx &= \int_{\mathbb{R}^d} \bar{u}(x) \sum_{k=1}^N x \cdot \left[\eta_k - \frac{2 + iB_k}{2L_k^2} x \right] u_k(x) dx \\ &= \sum_{k=1}^N \int_{\mathbb{R}^d} \bar{u}(x) \left[\eta_k \cdot x - \frac{2 + iB_k}{2L_k^2} |x|^2 \right] u_k(x) dx. \end{aligned}$$

Once again, this integral is computable thanks to the results of Appendix B.

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