Modulation algorithm for the Schrödinger equation

E. Faou, Y. Le Hénaff, P. Raphaël

Rennes University

Molecular Dynamics workshop

Angers, 21 Feb. 2024

Table of contents

Table of contents

Schrödinger equation

Linear Schrödinger equation, a.k.a. Quantum Harmonic Oscillator:

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

where $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$, $\Delta_x = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$, $\partial_t = \frac{\partial}{\partial t}$, $d \geq 1$.

Initial condition:

$$\psi(t=0,\cdot) = \psi_0 \quad \text{smooth enough.}$$

Numerical simulations

Main numerical algorithms

Numerical simulations

Main numerical algorithms :

- finite differences: most simple ones, also the most expensive. Not feasible in high dimension.

Numerical simulations

Main numerical algorithms :

- finite differences: most simple ones, also the most expensive. Not feasible in high dimension.
- grid-based spectral methods[1]: more accurate, but still rely on a grid.

[1] Joackim Bernier, Nicolas Crouseilles, and Yingzhe Li. "Exact Splitting Methods for Kinetic and Schrödinger Equations". In: *Journal of Scientific Computing* 86.1 (Jan. 2021).

Numerical simulations

Main numerical algorithms :

- finite differences: most simple ones, also the most expensive. Not feasible in high dimension.
- grid-based spectral methods: more accurate, but still rely on a grid.
- **gridless spectral methods**[1][2]: accurate and efficient depending on the initial condition.

[1] Weizhu Bao, Hailiang Li, and Jie Shen. "A Generalized-Laguerre–Fourier–Hermite Pseudospectral Method for Computing the Dynamics of Rotating Bose–Einstein Condensates". In: *SIAM Journal on Scientific Computing* 31.5 (Jan. 2009).

[2] Mechthild Thalhammer, Marco Caliari, and Christof Neuhauser. "High-Order Time-Splitting Hermite and Fourier Spectral Methods". In: *Journal of Computational Physics* 228.3 (Feb. 2009).

Numerical simulations

Main numerical algorithms :

- finite differences: most simple ones, also the most expensive. Not feasible in high dimension.
- grid-based spectral methods: more accurate, but still rely on a grid.
- **gridless spectral methods**: accurate and efficient depending on the initial condition.
- **variational methods**[1]: made for initial conditions that write as sum of complex Gaussian functions.

[1] Caroline Lasser and Christian Lubich. "Computing Quantum Dynamics in the Semiclassical Regime". In: *Acta Numerica* 29 (May 2020).

Gridless spectral methods

Idea: decompose the initial condition into an appropriate basis, then use the basis functions' properties to solve (QHO).

Gridless spectral methods

Idea: decompose the initial condition into an appropriate basis, then use the basis functions' properties to solve (QHO).

$$\psi(t,x) = \sum_{n\geq 0} c_n(t) H_n(x).$$

Gridless spectral methods

Idea: decompose the initial condition into an appropriate basis, then use the basis functions' properties to solve (QHO).

$$\psi(t,x) = \sum_{n\geq 0} c_n(t) H_n(x).$$

For instance, Hermite basis $\{H_n\}_{n\geq 0}$ is appropriate for (QHO) since

$$\begin{aligned} &(\Delta_x - |x|^2) H_n(x) = -(2n+1) H_n(x) \\ \Longrightarrow\ & i\partial_t c_n(t) = (2n+1) c_n(t). \end{aligned}$$

Gridless spectral methods

Idea: decompose the initial condition into an appropriate basis, then use the basis functions' properties to solve (QHO).

$$\psi(t,x) = \sum_{n\geq 0} c_n(t) H_n(x).$$

For instance, Hermite basis $\{H_n\}_{n\geq 0}$ is appropriate for (QHO) since

$$(\Delta_x - |x|^2) H_n(x) = -(2n+1) H_n(x)$$
$$\Longrightarrow i\partial_t c_n(t) = (2n+1) c_n(t).$$

Advantages: very efficient if the number of modes is small, easy to implement.

Drawbacks: Requiring an small number of modes in the basis imposes an implicit restriction at time $t = 0$. Example...

Gridless spectral methods

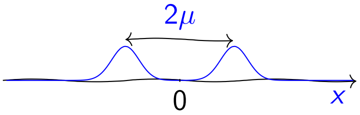
Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$

Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

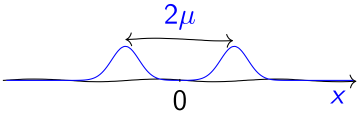
$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$

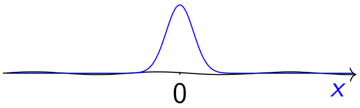


Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.

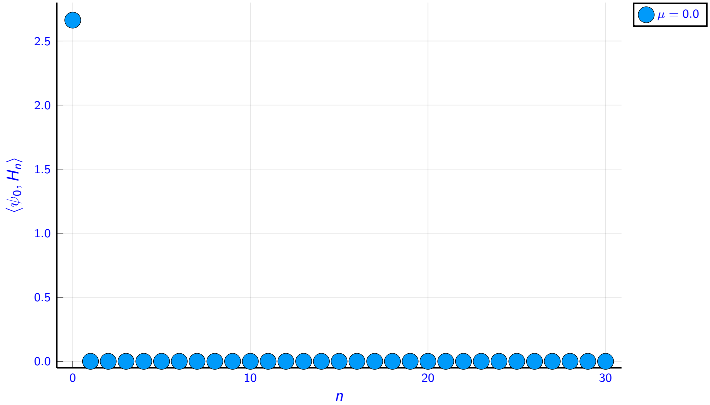
Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



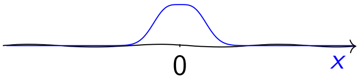
Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.



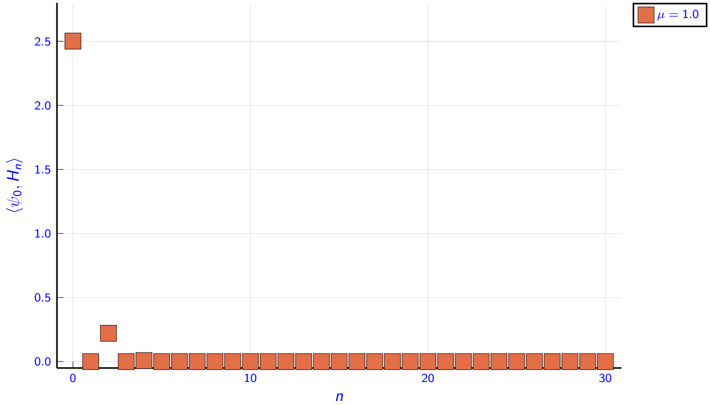
Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



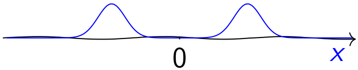
Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.



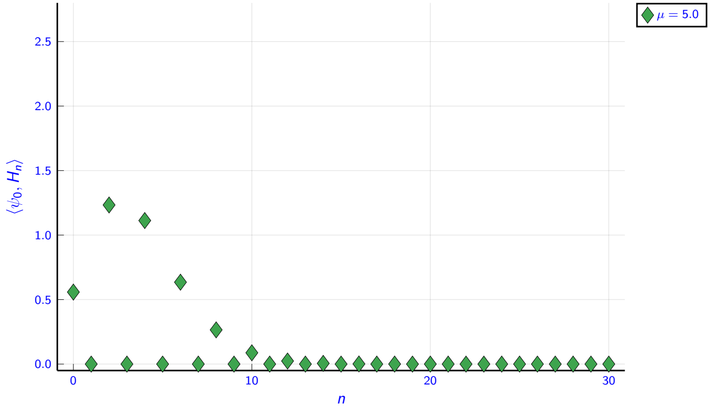
Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



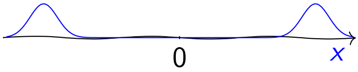
Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.



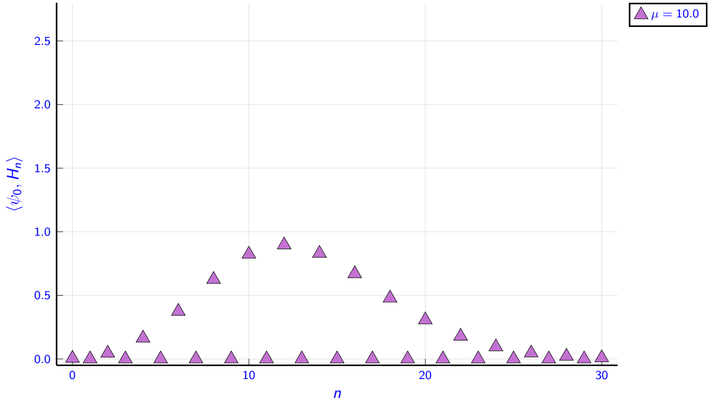
Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



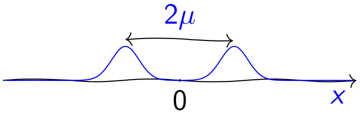
Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.



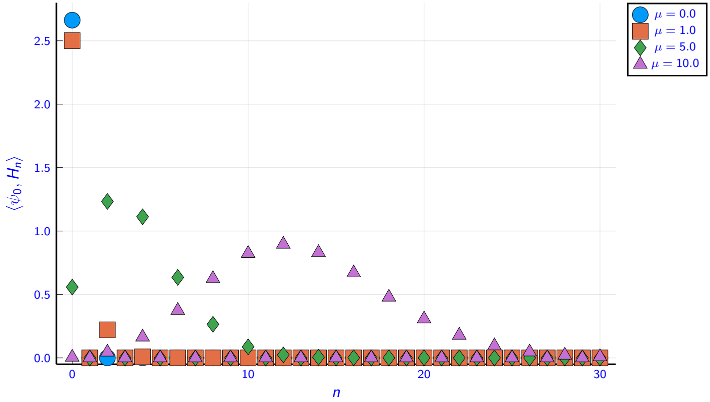
Gridless spectral methods

Solve (QHO) in dimension $d = 1$, where

$$\psi_0(x) = e^{-\frac{|x-\mu|^2}{2}} + e^{-\frac{|x+\mu|^2}{2}}, \quad \mu \in \mathbb{R}.$$



Appropriate basis: Hermite basis $\{H_n\}_{n\geq 0}$.



Variational methods

Variational methods

Use a variational principle on a sum of Gaussian functions.
Gaussian functions are very much liked because they are easy to deal with in this context.

Variational methods

Use a variational principle on a sum of Gaussian functions.
Gaussian functions are very much liked because they are easy to deal with in this context.
Either:

- Dirac-Frenkel variational principle: issues inherent to DFVP arise (non-invertibility of projection matrix), only ad-hoc procedure can help obtain satisfying results.

Variational methods

Use a variational principle on a sum of Gaussian functions.
Gaussian functions are very much liked because they are easy to deal with in this context.
Either:

- Dirac-Frenkel variational principle: issues inherent to DFVP arise (non-invertibility of projection matrix), only ad-hoc procedure can help obtain satisfying results.
- Rothe method: works better than DFVP, but requires solving nonlinear optimization problem at each timestep $\rightarrow$ expensive

Summary

Initial condition:

- sum of Gaussian functions $\rightarrow$ variational method
- few modes of a given basis $\rightarrow$ gridless spectral method

However, a Gaussian function is the first mode for Hermite basis $\rightarrow$ two possibilities in the simplest framework.

Proposed alternative: gridless spectral method designed for initial conditions as a sum of Gaussian functions $\rightarrow$ *modulation*.

Summary

Initial condition:

- sum of Gaussian functions $\rightarrow$ variational method
- few modes of a given basis $\rightarrow$ gridless spectral method

However, a Gaussian function is the first mode for Hermite basis $\rightarrow$ two possibilities in the simplest framework.

Proposed alternative: gridless spectral method designed for initial conditions as a sum of Gaussian functions $\rightarrow$ *modulation*.

Remark

More generally, we consider functions that write as a sum of few Hermite modes.

Table of contents

Modulation *ansatz*

Given $N \in \mathbb{N}^*$, decompose

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

with

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

where

$$y^j := \frac{x - X^j}{L^j}, \quad \text{and} \quad \frac{\mathrm{d}s^j}{\mathrm{d}t} := \frac{1}{(L^j)^2}. \quad \text{("bubble frame")}$$

Modulation *ansatz*

Given $N \in \mathbb{N}^*$, decompose

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

with

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

where

$$y^j := \frac{x - X^j}{L^j}, \quad \text{and} \quad \frac{\mathrm{d}s^j}{\mathrm{d}t} := \frac{1}{(L^j)^2}. \quad \text{("bubble frame")}$$

Modulation

All parameters depend on time!

Modulation *ansatz*

Given $N \in \mathbb{N}^*$, decompose

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

with

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

where

$$y^j := \frac{x - X^j}{L^j}, \quad \text{and} \quad \frac{\mathrm{d}s^j}{\mathrm{d}t} := \frac{1}{(L^j)^2}. \quad \text{("bubble frame")}$$

Modulation

All parameters depend on time!

Warning

No uniqueness of the decomposition (1), dictated by initial condition

Choice of parameters

By linearity, we plug each bubble u^j, into (QHO) (omit j index):

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

where $\Lambda v := y\cdot\nabla v$.

Choose parameters so that (QHO) appears again, in variables (s, y) with unknown v:

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

$\blacksquare = 0$, $\quad \blacksquare =$ -1.

ODEs to solve:

$$\begin{aligned} A_s &= \frac{AB}{2}(d-2), & L_s &= -BL \\ B_s &= -4 + 4L^4 - B^2, & X_s &= 2L^2\beta \\ \beta_s &= -2L^2 X, & \gamma_s &= L^2\left(|\beta|^2 - |X|^2\right). \end{aligned} \tag{5}$$

For each $j = 1, \dots, N$, v^j now satisfies (QHO) in bubble j's frame (s^j, y^j):

$$(i\partial_t + \Delta_x - |x|^2)u^j(t,x) = 0 \Longleftrightarrow (i\partial_{s^j} + \Delta_{y^j} - |y^j|^2)v^j(s^j, y^j) = 0$$

ODEs to solve:

$$
\begin{aligned}
A_s &= \frac{AB}{2}(d-2), & L_s &= -BL \\
B_s &= -4 + 4L^4 - B^2, & X_s &= 2L^2\beta \\
\beta_s &= -2L^2 X, & \gamma_s &= L^2\left(|\beta|^2 - |X|^2\right).
\end{aligned} \tag{5}
$$

For each $j = 1, \dots, N$, v^j now satisfies (QHO) in bubble j's frame (s^j, y^j):

$$(i\partial_t + \Delta_x - |x|^2)u^j(t,x) = 0 \iff (i\partial_{s^j} + \Delta_{y^j} - |y^j|^2)v^j(s^j, y^j) = 0$$

Miracle!

They can be integrated exactly!

Remark

They are the same equations as the Dirac-Frenkel variational principle when there is no redundancy in DFVP (i.e. no overlapping).

Explicit expressions of modulation parameters

$$A(t) = A(0)\left(\frac{L(t)}{L(0)}\right)^{\frac{2-d}{2}},$$

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

$$B(t) = 2\sin(\xi(t))\sqrt{4h(t)^2-1},$$

$$X_i(t) = \sin(\theta_i(t))\sqrt{2a_i(t)}, \quad i = 1,\dots,d,$$

$$\beta_i(t) = \cos(\theta_i(t))\sqrt{2a_i(t)}, \quad i = 1,\dots,d,$$

action-angle variables

$$a_i(t) = \frac{1}{2}\left(X_i(0)^2 + \beta_i(0)^2\right) = a_i(0),$$

$$\theta_i(t) = \arctan\left(\frac{X_i(0)}{\beta_i(0)}\right) + 2t,$$

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

$$\xi(t) = \arctan\left(\frac{B(0)}{4h(0) - 2L(0)^2}\right) - 4t.$$

$$\gamma(t) = \gamma(0) + \sum_{l=1}^{d}\frac{a_l(0)}{2}\left[\sin(2\theta_l(t)) - \sin(2\theta_l(0))\right]$$

$$s(t) = -\frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2-1}\right)\tan\left(\frac{\xi(0)}{2} - 2t\right)\right)$$
$$+\frac{1}{2}\arctan\left(\left(2h(0) + \sqrt{4h(0)^2-1}\right)\tan\left(\frac{\xi(0)}{2}\right)\right) + m_t\frac{\pi}{2},$$

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

Modulation parameters: OK. v?

Function v^j required to solve (QHO) in variables (s^j, y^j).

Hermite basis:

$$\left\{ \varphi_n(y^j) := H_{n_1}(y^j_1) \cdots H_{n_d}(y^j_d) : n \in \mathbb{N}^d \right\}.$$

Decompose

$$v^j(0, y^j) = \sum_{n \in \mathbb{N}^d} v^j_n \varphi_n(y^j), \tag{6}$$

with $v^j_n \in \mathbb{C}$, then

$$v^j(s^j, y^j) = \sum_{n \in \mathbb{N}^d} v^j_n e^{-(2|n|+d)is^j} \varphi_n(y). \tag{7}$$

Does it work well?

Reference scheme

In order to assess the efficiency of the bubble scheme, we need a reference scheme. We use a Fourier-spectral grid-based method with an exact splitting method between Δ and $|x|^2$ (cf.[2][3]):

$$e^{-it(-\Delta+|x|^2)} = e^{-\frac{i}{2}\tan(t)|x|^2} e^{\frac{i}{2}\sin(2t)\Delta_x} e^{-\frac{i}{2}\tan(t)|x|^2}.$$

Δ part approximated via a Fourier approach (with numerically truncated basis).

Two-dimensional examples, with 256 points used in each dimension, and a computational domain $[-15, 15] \times [-15, 15]$.

[2] Joackim Bernier, Nicolas Crouseilles, and Yingzhe Li. "Exact Splitting Methods for Kinetic and Schrödinger Equations". In: *Journal of Scientific Computing* 86.1 (Jan. 2021).

[3] Joackim Bernier. "Exact Splitting Methods for Semigroups Generated by Inhomogeneous Quadratic Differential Operators". In: *Foundations of Computational Mathematics* 21.5 (Oct. 2021).

Good properties of the bubble scheme

Numerical boundary conditions

The bubble scheme computes a solution on the unbounded domain $\mathbb{R}^d$!

Time evolution

In preparation of the third part of the presentation, results are shown at each timestep using time-discretization. **This is not necessary!** We can simply compute the bubble solution at time T, and doing a time-discretization just accumulates round-off errors.

Variational, gridless spectral, bubbles. . .

- gridless spectral method: $N = 1$
- variational method: N large

Assessing bubble scheme efficiency

Example 1: Video

$$\psi(t=0,x) = e^{-|x-\mu|^2} e^{i \cosh |x-\mu|} \approx e^{-|x-\mu|^2} e^{i + i \frac{|x-\mu|^2}{2}},$$

where $x \in \mathbb{R}^2$ and $\mu = (1,1)$.

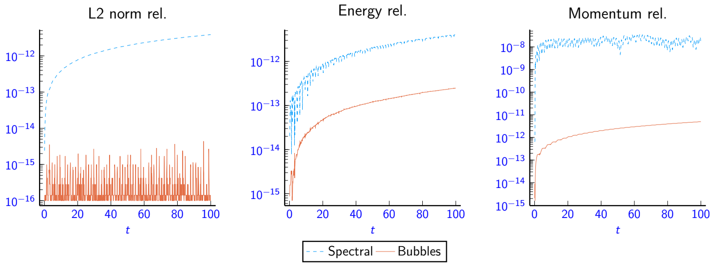


Figure: $\Delta t = 10^{-2}$.

Example 2: Video

$$\psi(t=0,x) = \sum_{i=1}^{3} e^{\gamma^j + i\beta^j \cdot (x - X^j) - \frac{|x-X^j|^2}{2(L^j)^2}},$$

$$\gamma^1 = 5 \qquad \gamma^2 = -5 \qquad \gamma^3 = 0,$$

$$X^1 = 7(1,0) \qquad X^2 = 7\left(-\frac{\sqrt{3}}{2}\right) \qquad X^3 = 7\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right),$$

with $L^j = 3$ and $\beta^j = (X^j)^\perp$, $j = 1,2,3$.

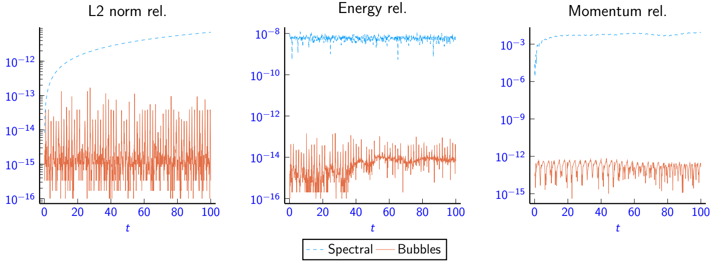


Figure: $\Delta t = 10^{-2}$.

Example 3: Video

$$\psi(t=0,x) = \pi e^{-\frac{|x-\mu_1|^2}{2L^2}} + 2e^{-\frac{|x-\mu_2|^2}{2L^2}}.$$

where $x \in \mathbb{R}^2$, $L = 2$, $\mu_1 = (0,5)$ and $\mu_2 = (8,0)$.

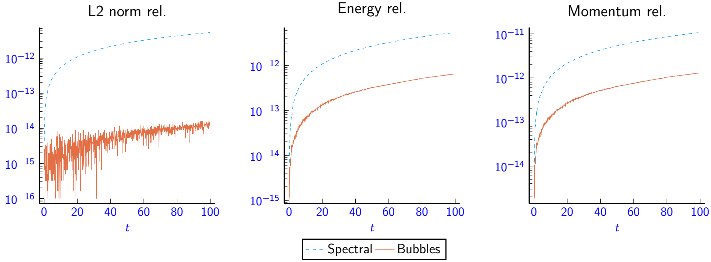


Figure: $\Delta t = 10^{-2}$.

Table of contents

We are now interested in the nonlinear Schrödinger equation:

$$i\partial_t u(t,x) + \Delta_x u(t,x) - |x|^2 u(t,x) = u(t,x)|u(t,x)|^2.$$

We now can solve (QHO) exactly, so by splitting, we only need to solve

$$i\partial_t u(t,x) = u(t,x)|u(t,x)|^2.$$

Restriction

We want to keep the bubble discretization

Simplifying assumption

We now consider $v^j(s^j, y^j) = \exp\left(-\frac{1}{2}|y^j|^2\right)$ (i.e. only first Hermite mode).

Simplifying assumption

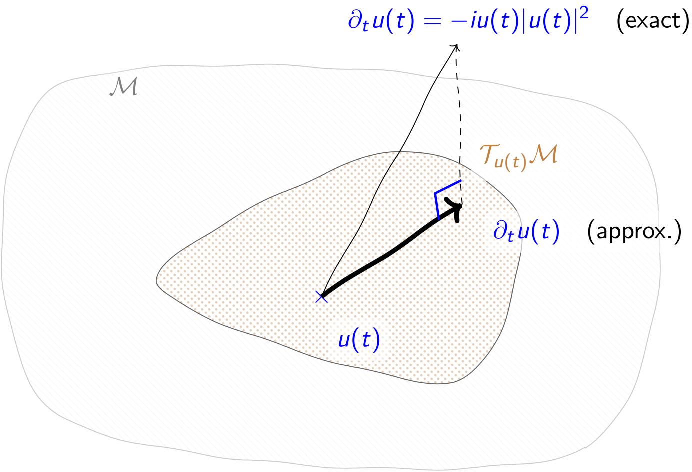
We now consider $v^j(s^j, y^j) = \exp\left(-\frac{1}{2}|y^j|^2\right)$ (i.e. only first Hermite mode).

Bubble decomposition: $u(t,\cdot) \in \mathcal{M}$, with

$$\mathcal{M} := \left\{ w \in \mathbb{L}^2(\mathbb{R}^d) \,\middle|\, \begin{array}{c} w(x) = \sum_{j=1}^{N} \frac{A^j}{L^j} e^{i\gamma^j + i\beta^j\cdot(x-X^j) - \frac{2+iB^j}{4(L^j)^2}\left|x-X^j\right|^2}, \\ A^j, B^j, \gamma^j \in \mathbb{R},\ L^j \in \mathbb{R}_+^*,\ X^j, \beta^j \in \mathbb{R}^d \end{array} \right\}. \quad (8)$$

We want to keep the bubble decomposition at all times, but $u(t,\cdot)|u(t,\cdot)|^2 \notin \mathcal{M} \to$ we project $\partial_t u(t)$ onto $\mathcal{M}$.

Dirac-Frenkel principle



Let $B_{u(t)}$ be a basis of $\mathcal{T}_{u(t)}\mathcal{M}$, then Dirac-Frenkel principle yields

$$\begin{aligned} &\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \quad \text{such that} \\ &\langle f, i\partial_t u(t)\rangle = \langle f, u(t)|u(t)|^2\rangle, \forall f \in B_{u(t)}. \end{aligned} \tag{9}$$

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

$$\begin{aligned} B_{u(t)} = \Big\{ & e^{i\Gamma^j(y^j) - \frac{|y|^2}{2}}, (y_1^j) e^{i\Gamma^j(y^j) - \frac{|y^j|^2}{2}}, \dots, (y_d^j) e^{i\Gamma^j(y^j) - \frac{|y^j|^2}{2}}, \\ & |y^j|^2 e^{i\Gamma^j(y^j) - \frac{|y^j|^2}{2}} : j = 1, \dots, N \Big\}, \end{aligned} \tag{10}$$

where we defined

$$\Gamma^j(y^j) := \gamma^j + L^j\beta^j \cdot y^j - \frac{B^j}{4}|y^j|^2.$$

Application of the Dirac-Frenkel principle results in a linear system:

$$\mathbf{AE} = \mathbf{S}.$$

The vector $\mathbf{E}$ contains approximate time derivatives of each parameter.

Computation of $\mathbf{A}$ and $\mathbf{S}$

We use analytical formulas for the components of $\mathbf{A}$ and $\mathbf{S}$, since their components are product of Gaussian in different frames. Should also be doable with Hermite functions, we did not try yet to do the computations. For more general functions v, need to resort to numerical integration.

Does it work well?

Assessing bubble scheme efficiency

Example 1: Video

$$\psi(t=0,x) = e^{-|x-\mu|^2} e^{i\cosh|x-\mu|} \approx e^{-|x-\mu|^2} e^{i+i\frac{|x-\mu|^2}{2}},$$

where $x \in \mathbb{R}^2$ and $\mu = (1,1)$.

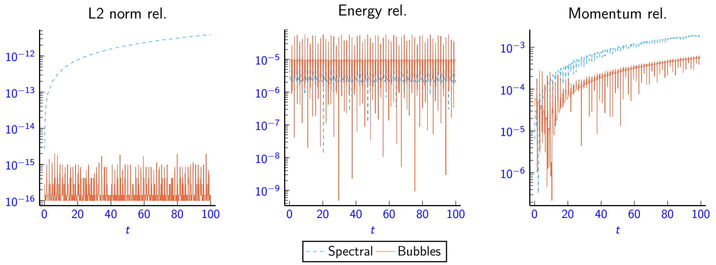


Figure: $\Delta t = 10^{-2}$.

Example 2: Video

$$\psi(t=0,x) = \sum_{i=1}^{3} e^{\gamma^j + i\beta^j\cdot(x-X^j) - \frac{|x-X^j|^2}{2(L^j)^2}},$$

$$\gamma^1 = 5 \qquad \gamma^2 = -5 \qquad \gamma^3 = 0,$$

$$X^1 = 7(1,0) \qquad X^2 = 7\left(-\frac{\sqrt{3}}{2}\right) \qquad X^3 = 7\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right),$$

with $L^j = 3$ and $\beta^j = (X^j)^\perp$, $j = 1, 2, 3$.

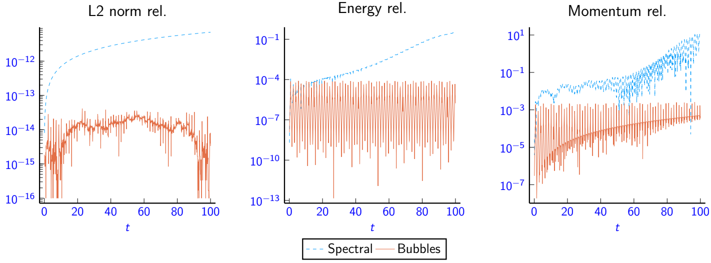


Figure: $\Delta t = 10^{-2}$.

Example 3: Video

$$\psi(t=0,x) = \pi e^{-\frac{|x-\mu_1|^2}{2L^2}} + 2e^{-\frac{|x-\mu_2|^2}{2L^2}}.$$

where $x \in \mathbb{R}^2$, $L = 2$, $\mu_1 = (0,5)$ and $\mu_2 = (8,0)$.

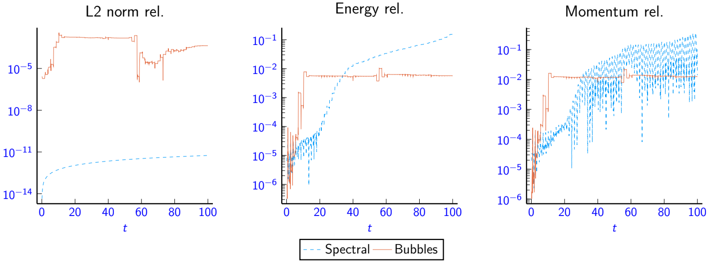


Figure: $\Delta t = 10^{-2}$.

Remarks

Modulation works very well in the linear setting Dirac-Frenkel principle works well when $\mathbf{A}$ is well-conditioned.

When it is not the case, the approximation is very bad and yields very large time derivative of parameters $\rightarrow$ jumps observed. It is inherent to the Dirac-Frenkel principle $\rightarrow$ Loïc's work?

Thank you for your attention!

References

[1] Joackim Bernier, Nicolas Crouseilles, and Yingzhe Li. "Exact Splitting Methods for Kinetic and Schrödinger Equations". In: *Journal of Scientific Computing* 86.1 (Jan. 2021).

[2] Weizhu Bao, Hailiang Li, and Jie Shen. "A Generalized-Laguerre–Fourier–Hermite Pseudospectral Method for Computing the Dynamics of Rotating Bose–Einstein Condensates". In: *SIAM Journal on Scientific Computing* 31.5 (Jan. 2009).

[3] Mechthild Thalhammer, Marco Caliari, and Christof Neuhauser. "High-Order Time-Splitting Hermite and Fourier Spectral Methods". In: *Journal of Computational Physics* 228.3 (Feb. 2009).

[4] Caroline Lasser and Christian Lubich. "Computing Quantum Dynamics in the Semiclassical Regime". In: *Acta Numerica* 29 (May 2020).

[5] Joackim Bernier. "Exact Splitting Methods for Semigroups Generated by Inhomogeneous Quadratic Differential Operators". In: *Foundations of Computational Mathematics* 21.5 (Oct. 2021).