Some effect of discretization in Hamiltonian PDEs

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Linear systems and time integration

- Hamiltonian linear systems :

$$\partial_t y = iAy \qquad y \in \mathbb{C}^N, \qquad A^* = A.$$

- Preservation of the energy $y^* Ay = \langle y|A|y\rangle \in \mathbb{R}$.
- Solutions oscillate at the frequencies of the matrix

$$A = Q^*\Omega Q, \quad Q^*Q = I, \quad \Omega = \mathrm{diag}(\omega_k), \quad \omega_k \in \mathbb{R}.$$

$$\begin{aligned} y(t) = \exp(itA)y(0) &= Q^*\mathrm{diag}(\exp(it\omega_k))Q\,y(0) \\ &= \sum_{k=1}^{N} \exp(it\omega_k) z_k^0. \end{aligned}$$

- Stability for all times : $\|y(t)\| \le C$.

Linear systems and time integration

Time integration : $y_n \simeq y(\tau n) = \exp(i\tau n A)y(0)$.

$$\left| \begin{array}{ll} y_{n+1} = y_n + i\tau A y_n, & \textit{Euler} \\ y_{n+1} = y_n + i\tau A\left(\dfrac{y_n + y_{n+1}}{2}\right) & \textit{Midpoint rule} \end{array} \right.$$

In both case

$$y_{n+1} = \phi(i\tau A)y_n \quad \left| \begin{array}{ll} \phi(z) = 1 + z & \textit{Euler} \\ \phi(z) = \dfrac{1+\frac{z}{2}}{1-\frac{z}{2}} & \textit{Midpoint rule} \end{array} \right.$$

$$A = Q^*\Omega Q \Longrightarrow \phi(i\tau A) = Q^*\phi(i\tau\Omega)Q \Longrightarrow y_n = Q^*\phi(i\tau\Omega)^n Q\, y(0).$$

Hence we have an approximation

$$\exp(i\tau n\omega_k) \simeq \phi(i\tau\omega_k)^n = \left| \begin{array}{ll} (1 + i\tau\omega_k)^n & \textit{Euler} \\ \left(\dfrac{1 + i\frac{\tau\omega_k}{2}}{1 - i\frac{\tau\omega_k}{2}}\right)^n & \textit{Midpoint rule} \end{array} \right.$$

Linear systems and time integration

Stability problem :

$$|\exp(i\tau\omega_k)| = 1, \quad |1 + i\tau\omega_k| > 1, \quad \left|\frac{1 + i\frac{\tau\omega_k}{2}}{1 - i\frac{\tau\omega_k}{2}}\right| = 1$$

$$\|y(t)\| \leq C, \quad \text{but} \quad \left| \begin{array}{lll} \|y_n\| \underset{n\to\infty}{\longrightarrow} +\infty & & \textit{Euler} \\ \|y_n\| \leq C & \forall\, n & \textit{Midpoint rule.} \end{array} \right.$$

Shadow equation :$y_{n+1} = \exp(i\tau\frac{1}{i\tau}\log(\phi(i\tau A)))y_n$.

Numerically, we see the exact solution of

$$\dot{y} = \left(\frac{1}{i\tau}\log\phi(i\tau A)\right)y = A_\tau y \qquad \left| \begin{array}{ll} A_\tau = \dfrac{1}{i\tau}\log(1 + i\tau A) & \textit{Euler} \\ A_\tau = \dfrac{2}{\tau}\arctan(\dfrac{\tau A}{2}) & \textit{Midpoint rule.} \end{array} \right.$$

$$\frac{1 + ix}{1 - ix} = \exp(2i\arctan(x)). \qquad A_\tau^* = A_\tau \quad \text{for midpoint.}$$

Linear systems and time integration

Time integration : Modified equation

$$\dot{y} = iAy \quad \underset{\text{time grid}}{\Longrightarrow} \quad \dot{y} = iA_\tau y$$

- A_τ symmetric if and only if the method is symplectic
- Symplectic methods are always implicit and stable.
  RK4 not symplectic.
- Order of the method : $\|A - A_\tau\| = \mathcal{O}(\tau^p)$.
- High Frequencies are smoothed

$$\omega_k \xrightarrow[k\to\infty]{} \infty \quad \text{but} \quad \omega_{k,\tau} = \frac{2}{\tau}\arctan\left(\frac{\tau\omega_k}{2}\right) \leq \frac{\pi}{\tau} \quad \forall k.$$

  Always a difference between exact frequencies and numerical frequencies, except when A is diagonal or easily diagonalizable.
- Modified energy $\langle y|A_\tau|y\rangle$ preserved for all times.

Splitting and modified energy

$$\partial_t y = iAy + iBy, \qquad A, B \text{ symmetric}$$

- Exact flow : $u(t) = \exp(it(A+B))u^0$
- Splitting methods : order 1 (Lie)

$$y_{n+1} = \exp(i\tau A)\exp(i\tau B)y_n = \exp(i\tau(A+B))y_n + \mathcal{O}(\tau^2)$$

- Order 2 (Strang, Störmer-Verlet)

$$y_{n+1} = \exp(i\frac{\tau}{2}A)\exp(i\tau B)\exp(i\frac{\tau}{2}A)y_n = \exp(i\tau(A+B))y_n + \mathcal{O}(\tau^3)$$

- Idea : $\exp(i\tau A)$ and $\exp(i\tau B)$ easy to compute.
  Typically : A operator diagonal in frequency,
  B multiplication potential. Inbetween : FFT.

Splitting and modified energy

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

Baker-Campbell-Haussdorf formula

$$\exp(i\tau A) \circ \exp(i\tau B) = \exp(iZ(\tau))$$

$$Z(\tau) = \tau(A + B) + \tfrac{1}{2} i\tau^2 [A, B] + \cdots$$

- $[A, B] = AB - BA =: \mathrm{ad}_A(B)$
- Convergence of the series for $\tau(\|A\| + \|B\|) < 2\pi$.
- Modified energy :

$$\langle y | \frac{1}{\tau} Z(\tau) | y \rangle = \langle y | A + B | y \rangle + \mathcal{O}(\tau).$$

Linear Hamiltonian PDEs

Main examples : Schrödinger equations. $u(t,x)$ solution of

$$iu = -\Delta u \qquad x \in \mathbb{T}^d \qquad \textit{Torus}$$

$$iu = Hu = (-\Delta + |x|^2)u \qquad x \in \mathbb{R}^d \qquad \textit{Full space}$$

To define the solution : diagonalization of the operators

$$\left| \begin{array}{lll} -\Delta e^{ik\cdot x} = |k|^2 e^{ik\cdot x} & k \in \mathbb{Z}^d, & \textit{Plane waves in } \mathbb{T}^d \\ H\varphi_n = (2|n| + d)\varphi_n = \omega_n \varphi_n & n \in \mathbb{N}^d, & \textit{Hermite functions on } \mathbb{R}^d. \end{array} \right.$$

Solution preserve the Sobolev norms H^s (torus) or
$\mathcal{H}^s = \{u \,|\, \langle x\rangle^s u \in L^2, \quad \langle \nabla \rangle^s u \in L^2\}$ (harmonic oscillator).

$$\left| \begin{array}{lll} u(t) = \sum_{k\in\mathbb{Z}^d} e^{-it|k|^2} \hat{u}_k^0 e^{itk\cdot x} & \hat{u}_k^0 & \textit{Fourier transform of} \quad u^0 \\ u(t) = \sum_{n\in\mathbb{N}^d} e^{-it\omega_n} u_n^0 \varphi_n(x) & u_n^0 & \textit{Hermite transform of} \quad u^0. \end{array} \right.$$

Linear Hamiltonian PDEs : Space and time discretization

Finite differences on $\mathbb{T}^d$.

Space grid $x_j = jh$ on $\mathbb{T}^d$, $K \simeq 1/h$ points.

$$i\partial_t u = -\Delta u \quad \underset{\text{space grid}}{\Longrightarrow} \quad i\partial_t u_j = -\frac{u_{j+1} - 2u_j + u_{j-1}}{h^2}$$

$$i\dot{y} = A_h y, \quad A_h = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad \text{with} \quad y = (u_j) \in \mathbb{C}^K.$$

Eigenvalue of the matrix : $|k|^2 \sim \frac{4}{h^2}\sin^2(\frac{h|k|^2}{2})$. After time discretization

$$\dot{y} = A_{\tau,h} y, \quad |k|^2 \sim \left| \begin{array}{ll} \frac{2}{\tau}\arctan(\frac{2\tau}{h^2}\sin^2(\frac{h|k|^2}{2})) & \textit{midpoint} \\ \omega_{\tau,h,k} + i\gamma_{\tau,h,k} & \textit{Explicit method } \gamma_{\tau,h,k} \neq 0. \end{array} \right.$$

Linear Hamiltonian PDEs : Space and time discretization

Spectral methods. Grid $x_j = jh$ on $\mathbb{T}^d$, $K \simeq 1/h$ points.

$$u(t,x) \simeq \sum_{k\in\{\frac{K-1}{2},\dots,\frac{K}{2}\}} e^{ik\cdot x} u_k^K(t)$$

- After discrete FFT on the grid x_j, the equation is

$$\forall\, k \qquad i\partial_t u_k^K(t) = |k|^2 u_k^K(t) \quad \text{diagonal matrix.}$$

  Exact up to spectral approximation.
- On $\mathbb{R}^d$: we embed in a large torus of size L.
  (or with Dirichlet boundary condition)
  And hope for not to much error... (boundary effects)
- Advantage : Easy to switch from the frequency space to the physical space $\mathcal{O}(K \log K)$ operation (potential evaluation, nonlinearity).

Linear Hamiltonian PDEs : Space and time discretization

- Problem with the Harmonic oscillator : No Fast Hermite transform.

$$u(t,x) \simeq \sum_{n\in\{0,\dots,K\}} \varphi_n(x) u_n^K(t)$$

The "Hermite grids" are not included and change when K vary.
No divide and conquer algorithm.

- Idea of splitting ?

$$e^{-i\tau H} \simeq e^{-i\frac{\tau}{2}|x|^2} e^{i\tau\Delta} e^{-i\frac{\tau}{2}|x|^2}$$

but Δ and $|x|^2$ are operator of the same order : Large error .

- Quadratic evolution operator : Bernier splitting of the form

$$e^{-itH} = e^{i\alpha(t)|x|^2} e^{i\beta(t)\Delta} e^{i\gamma(t)|x|^2}$$

Exact with explicit formulas for $\alpha(t), \beta(t)$... Using FFT $\mathcal{O}(K\log K)$
Preliminary results by Blanes & Bader (2018), full generalization by Joackim Bernier (2020) for any quadratic operator.
Only error comes from the large torus approximation.

A numerical example

Focusing Schrödinger equation on $\mathbb{R}$

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

- Preservation of the L^2 norm $\|u(t)\|_{L^2}^2 = \|u(0)\|_{L^2}^2$ and of the energy

$$H(u) = \int_{\mathbb{R}} |\partial_x u(x)|^2 - \frac{1}{2}|u(x)|^4 \mathrm{d}x = T(u) + P(u)$$

- Pseudospectral discretisation : Large torus $\mathbb{T}_L = \mathbb{R}/(2\pi L\mathbb{Z})$.

$$\varphi_T^t(u) = e^{it\Delta}u \qquad (\varphi_P^t(u))(x) = e^{it|u(x)|^2}u(x)$$

  Two parts are "explicit" up to FFT and space discretization.

- Splitting schemes : For small τ,

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq \phi_T^\tau \circ \phi_P^\tau, \quad \Longrightarrow \phi_H^{n\tau}(u^0) \simeq \left(\phi_T^\tau \circ \phi_P^\tau\right)^n (u^0).$$

Solitary waves

$$i\partial_t u(t,x) = -\partial_{xx} u(t,x) - |u(t,x)|^2 u(t,x), \quad u(0,x) = u^0(x), \quad x \in \mathbb{R}.$$

- Family of solutions (solitary waves)

$$u(t,x) = \rho(x - ct - x_0) \exp(i(\frac{1}{2}c(x - ct - x_0) + \theta_0)) \exp(i(a + \frac{1}{4}c^2)t)$$

  a, c, x_0 and θ_0 are real parameters,

$$\rho(x) = \frac{\sqrt{2a}}{\cosh(\sqrt{a}x)}.$$

- Stable solitons (orbital stability)
- Very particular solution :

$$u(t,x) = \frac{\sqrt{2}e^{it}}{\cosh(x)}.$$

Solitary waves

- Space discretization : large window $[-\pi/\sigma, \pi/\sigma]$ (σ small). Fourier pseudo spectral methods with K equidistant points.
- First case : Explicit splitting method.

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq \phi_T^\tau \circ \phi_P^\tau$$

- $K = 256$, $\sigma = 0.11$. Courant-Friedrichs-Lewy number :

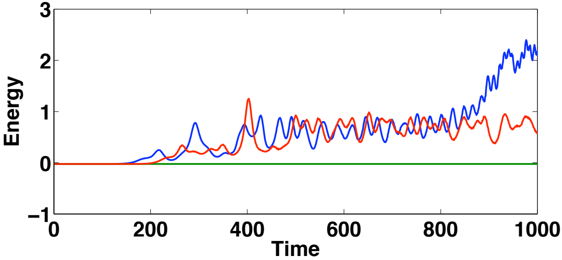
$$\mathrm{cfl} = \tau\sigma^2\Big(\frac{K}{2}\Big)^2.$$

  - $\tau = 0.1$ (cfl = 19.8),
  - $\tau = 0.05$ (cfl = 9.9),
  - $\tau = 0.01$ (cfl = 1.9).

Solitary waves

Evolution of the energy

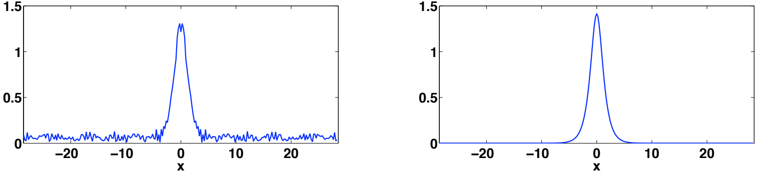
$$H(u,\bar{u}) = \int_{\mathbb{R}} |\partial_x u(x)|^2 - \frac{1}{2}|u(x)|^4 \mathrm{d}x$$



- $\tau = 0.1$ (cfl = 19.8) : Energy drift
- $\tau = 0.05$ (cfl = 9.9) : Energy drift
- $\tau = 0.01$ (cfl = 1.9) : No drift.

Solitary waves

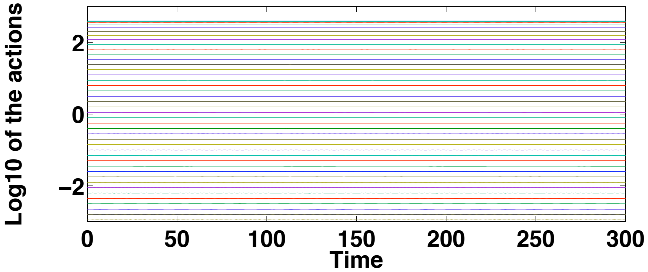
Profile of the solution : $|u^n(x)|$



- cfl $= 19.8$ at time $t = 300$ (left)
- cfl $= 1.9$ at time $t = 10000$ (right)

Solitary waves

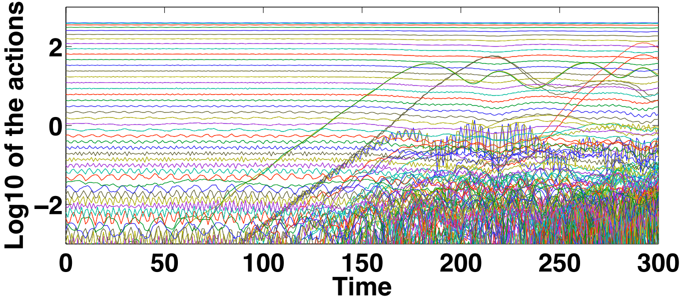
Plot of the Fourier coefficients $|\hat{u}_k(t)|^2$ for $k \in \mathbb{Z}$ in log scale.



First case : cfl $= 1.9$

Solitary waves

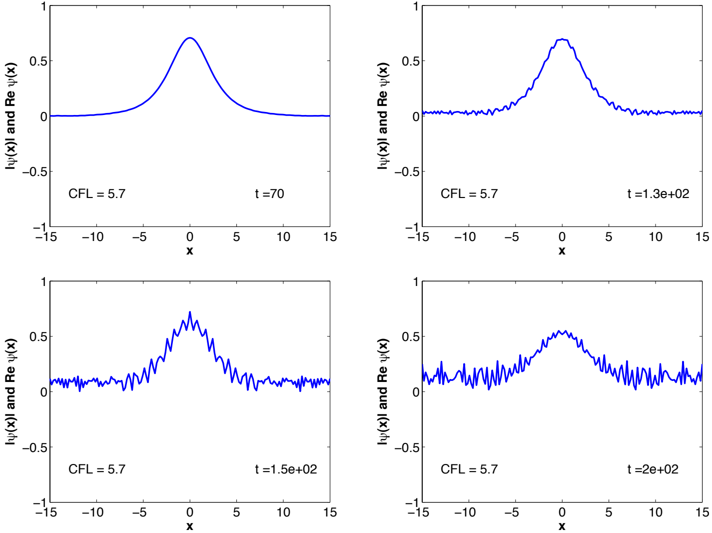
Plot of the Fourier coefficients $|\hat{u}_k(t)|^2$ for $k \in \mathbb{Z}$ in log scale.



Second case : cfl $= 19.8$. Leak of energy in the high modes.

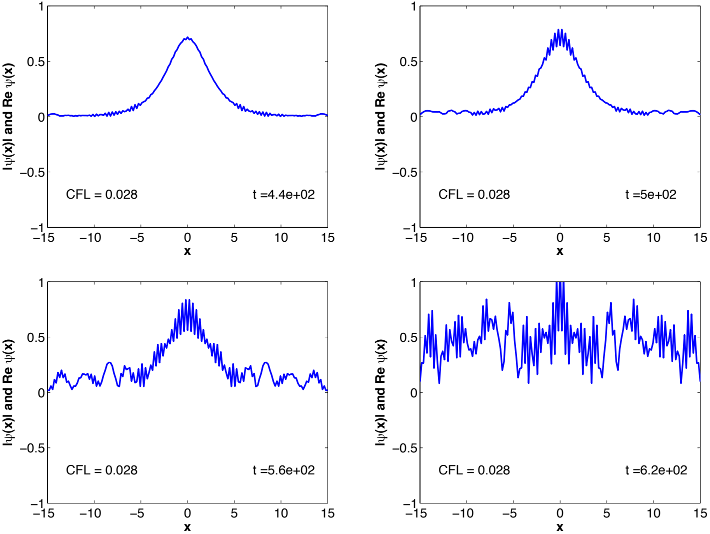
Solitary waves

Symplectic splitting, cfl $= 5.7$.



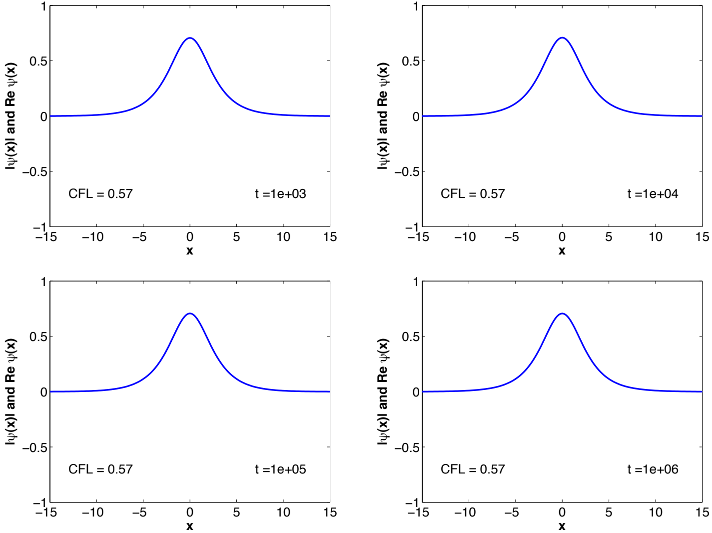
Solitary waves

Non symplectic integrators : $\exp(\tau A) \simeq I + \tau A + \frac{\tau^2}{2} A^2$, cfl $= 0.028$.



Solitary waves

Symplectic splitting : cfl $= 0.57$.



Solitary waves

Same computation with the implicit-explicit (IMEX) integrator :

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq R(i\tau\Delta) \circ \phi_P^\tau$$

with

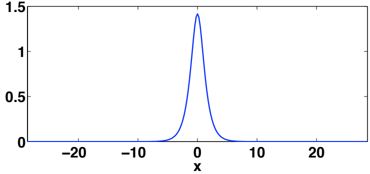
$$R(i\tau\Delta) = \frac{1 + i\tau\Delta/2}{1 - i\tau\Delta/2} \simeq \exp(i\tau\Delta)$$

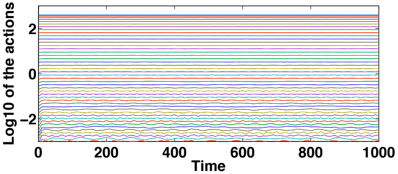
Midpoint rule applied to the free Schrödinger equation

$$i\partial_t u = -\Delta u \quad \Longrightarrow u^{n+1} = u^n + i\tau\Delta\Big(\frac{u^{n+1} + u^n}{2}\Big)$$

We use $\mathrm{cfl} = 19.8$.

Solitary waves





No energy drift, preservation of the regularity, even with cfl $= 19.8$.
Results for discrete solitons :

- Symmetric case : Bambusi & Penati (2010) (space discretization), Bambusi, Faou & Grébert (2013)
- Moving discrete solitary waves : Bernier & Faou (2019)
- CFL condition must always be imposed, except for some energy preserving schemes (Delfour, Fortin & Payre (1981)).
- Weinstein conjecture ?

Backward error analysis : principles

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

- A and B real operators (possibly unbounded, possibly nonlinear)
- Exact flow : $u(t) = \exp(it(A+B))u^0$
- Splitting methods

$$u^1 = \exp(i\tau A) \circ \exp(i\tau B) u^0 = u(\tau) + \mathcal{O}(\tau^2)$$

- Global order 1, Existence of high order splitting.
- preservation of the L^2 norm
- Convergence in H^s under smoothness assumption in $H^{s+\eta}$ (for finite times).

Backward error analysis : principles

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

Baker-Campbell-Haussdorf formula

$$\exp(i\tau A) \circ \exp(i\tau B) = \exp(iZ(\tau))$$

$$Z(\tau) = \tau(A + B) + \frac{1}{2} i\tau^2 [A, B] + \cdots$$

- Convergence of the series for $\tau(\|A\| + \|B\|) < 2\pi$.
  $A = -\Delta$ or $A = H$: no convergence to hope.

$$\| \exp(i\tau A) \circ \exp(i\tau B) y - \exp(i\tau(A + B)) y \|_{L_2} = \mathcal{O}(\tau^N \|y\|_{H^{2N}}).$$

Need an a posteriori bound of the numerical solution in all the H^s.
Not true in general.

BCH with unbounded part

$A = -\Delta$, writing $\exp(i\tau A) = I + i\tau A - \frac{\tau^2}{2}A^2 + \cdots$ not an option.

$$\exp(i\tau A) \circ \exp(i\tau B) = \exp(iZ_0) \circ \exp(i\tau B) = \exp(iZ(\tau))??$$

- $Z_0 = \mathrm{diag}(\lambda_k)$ bounded but not small.
- Explicit integrators : $\lambda_k = \tau|k|^2$ modulo 2π in Fourier.

$$\exp(-i\tau\Delta) = \mathrm{diag}(\exp(i\tau|k|^2))$$

- implicit-explicit integrators : $\lambda_k = 2\arctan(h|k|^2/2)$

$$R(-i\tau\Delta) = \frac{1 - i\tau\Delta/2}{1 + i\tau\Delta/2} = \exp(2i\arctan(-\tau\Delta/2)) =: \exp(iZ_0).$$

BCH with unbounded part

Find $Z(t)$ such that

$$\forall\, t \in [0,\tau], \quad \exp(iZ_0) \circ \exp(itB) = \exp(iZ(t)), \quad Z(0) = Z_0.$$

Equation

$$Z'(t) = (\mathrm{d}\exp_{iZ(t)})^{-1} \exp(-iZ(t))B = \sum_{n\geq 0} \frac{B_n}{n!} \mathrm{ad}^n_{iZ(t)}(B).$$

- B_n Bernoulli numbers. $\displaystyle\sum_{n=0}^{\infty} \frac{B_n}{n!} x^n = \frac{x}{e^x - 1}$.
- Expansion : $Z(t) = Z_0 + tZ_1 + \cdots$
- Second term :

$$Z_1 = \sum_{n\geq 0} \frac{B_n}{n!} i^k \mathrm{ad}^n_{Z_0}(B).$$

Nonlinear case : $\mathrm{ad}_H(K) = \{H, K\}$ (Hamiltonian).

Linear Schrödinger equation

$$\partial_t u(t,x) = -i\Delta u(t,x) + iV(x)u(t,x), \quad u(0,x) = u_0(x).$$

- $x \in \mathbb{T}^d$. In Fourier $A = -\Delta = \mathrm{diag}(|k|^2)$. $B = (\widehat{V}_{k-\ell})_{k,\ell\in\mathbb{Z}^d}$.
- $Z_0 = \mathrm{diag}(\lambda_k)$ with $\lambda_k = \tau|k|^2$ or $\lambda_k = 2\arctan(\tau|k|^2/2)$.

$$\begin{aligned}\left(\mathrm{ad}_{Z_0} W\right)_{k\ell} &= \big((Z_0)_{kk} - (Z_0)_{\ell\ell}\big)W_{k\ell},\\ &= \big(\lambda_k - \lambda_\ell\big)W_{k\ell}.\end{aligned}$$

- $(Z_1)_{k\ell} = B_{k\ell}\dfrac{i(\lambda_k - \lambda_\ell)}{\exp(i(\lambda_k - \lambda_\ell)) - 1}$ well defined for $|\lambda_k - \lambda_\ell| < 2\pi$

Modified energy

Theorem (Debussche & Faou 2008)

For the implicit-explicit integrator, there exists a symmetric operator $S(\tau)$ such that for all $\tau \leq \tau_0$

$$R(-i\tau\Delta)\exp(i\tau V) = \exp(i\tau S(\tau))$$

Moreover

$$S(\tau) = \frac{2}{\tau}\arctan(-\tau\Delta/2) + \tilde{V}(\tau)$$

- $\tilde{V}(\tau)$ modified (bounded and smooth) potential
- $\langle u|S(\tau)|u\rangle$ invariant of the numerical scheme
- No residual term.
- Backward error analysis result.
- Same result for explicit splitting with CFL.

Modified energy

$$S(\tau) = \frac{2}{\tau}\arctan(-\tau\Delta/2) + \tilde{V}(\tau)$$

We have for the numerical solution u^n :

$$\langle u^n | S(\tau) | u^n \rangle = \langle u^0 | S(\tau) | u^0 \rangle$$

Corollary

for all n we have

$$\sum_{|k|\le 1/\sqrt{\tau}} |k|^2 |u_k^n|^2 + \frac{1}{\tau} \sum_{|k|>1/\sqrt{\tau}} |u_k^n|^2 \le C_0 \| u^0 \|_{H^1}^2 .$$

- Fully discrete system : aliasing problems
- Under CFL conditions : H^1 bounds of the solution independent on K.

Cubic nonlinear Schrödinger equation

$$i\partial_t u = -\Delta u + |u|^2 u = \frac{\partial H}{\partial \bar{u}}(u, \bar{u})$$

Wave function $u(t,x) \in \mathbb{C}$, $x \in \mathbb{T}$.

- Hamiltonian

$$H(u, \bar{u}) = \int_{\mathbb{T}} (|\nabla u|^2 + \frac{1}{2}|u|^4)\mathrm{d}x.$$

- Decomposition $u = \sum_{k\in\mathbb{Z}} u_k e^{ikx}$,

$$\begin{aligned} H(u,\bar{u}) &= T(u,\bar{u}) + P(u,\bar{u}) \\ &= \sum_{k\in\mathbb{Z}} |k|^2 |u_k|^2 + \frac{1}{2} \sum_{k+m-\ell-j=0} u_k u_m \bar{u}_\ell \bar{u}_j. \end{aligned}$$

Cubic nonlinear Schrödinger equation

- Hamiltonian system : for all $k \in \mathbb{Z}$,

$$\dot{u}_k = -i|k|^2 u_k - i \sum_{k=k-\ell+m} u_k \bar{u}_\ell u_m.$$

- $A = -\Delta$, $B = P$ Polynomial Hamiltonian P

$$P = \frac{1}{2} \sum_{k+m-\ell-j=0} u_k u_m \bar{u}_\ell \bar{u}_j$$

Action of $Z_0 = \sum_k \lambda_k |u_k|^2$:

$$\{Z_0, u_k u_m \bar{u}_\ell \bar{u}_j\} = i\Omega_{km\ell j} u_k u_m \bar{u}_\ell \bar{u}_j$$

where

$$\Omega_{km\ell j} = \lambda_k + \lambda_m - \lambda_\ell - \lambda_j$$

Modified energy

First term :

$$Z_1 = \frac{1}{2} \sum_{k+m-\ell-j=0} \left(\frac{i\Omega_{km\ell j}}{e^{i\Omega_{km\ell j}} - 1} \right) u_k u_m \bar{u}_\ell \bar{u}_j$$

- Z_1 : Control of the small denominator at the order 4.
- Z_2 : defined similarly, but of degree 6.
- Construction of Z_n : $\lambda_k \leq \frac{2\pi}{n+1}$.
- In general : CFL condition $\tau |k|^2 \leq \frac{2\pi}{n+1}$ or $\tau |k|^2 \leq 2 \tan(\frac{\pi}{n+1})$

Modified flow

Theorem (Faou & Grébert 2009)

There exists a polynomial Hamiltonian H_τ *such that for all* $u \in B_M = \{ u \in \ell^1 \,|\, \|u\|_{\ell^1} \leq M \}$, *we have*

$$\|\phi_P^\tau \circ \phi_{Z_0}^1(u) - \phi_{H_\tau}^\tau(u)\|_{\ell^1} \leq \tau^{N+1}(CN)^N.$$

In general, N *is given by the CFL condition.* $\|u\|_{\ell^1} := \sum_{k\in\mathbb{Z}} |u_k|$.

$$H_\tau(u,\bar{u}) = \sum_{k\in\mathbb{Z}} \frac{1}{\tau}\lambda_k |u_k|^2 + \frac{1}{2}\sum_{k+m-\ell-j=0} \frac{i\Omega_{km\ell j}}{e^{i\Omega_{km\ell j}} - 1} u_k u_m \bar{u}_\ell \bar{u}_j + \mathcal{O}(\tau)$$

CFL conditions

Splitting or implicit explicit method : CFL condition
For cubic NLS : cfl numbers

τ^{N+1}	x	$2\arctan(x/2)$
τ^2	3.14	∞
τ^3	2.10	3.46
τ^4	1.57	2.00
τ^5	1.27	1.45
τ^6	1.05	1.15
τ^7	0.90	0.96
τ^8	0.80	0.83
τ^9	0.70	0.73
τ^{10}	0.63	0.65

Fully discrete case

The discretized Hamiltonian writes (in dimension 1)

$$\sum_{k\in B_K} |k|^2|u_k|^2 + \frac{1}{2} \sum_{\substack{k,m,\ell,j\in B_K^4 \\ k+m-\ell-j\in K\mathbb{Z}}} u_k u_m \bar{u}_\ell \bar{u}_j.$$

where $B_K = \{j \in \mathbb{Z} \,|\, -\frac{K}{2} \le j \le \frac{K}{2} - 1\}$.
Modified Hamiltonian for the explicit splitting with CFL $(\lambda_k = \tau|k|^2)$.

$$H_\tau(u,\bar{u}) = \sum_{k\in B_K} |k|^2|u_k|^2 + \frac{1}{2} \sum_{\substack{k,m,\ell,j\in B_K^4 \\ k+m-\ell-j\in K\mathbb{Z}}} \frac{i\Omega_{km\ell j}(\tau)}{e^{i\Omega_{km\ell j}(\tau)} - 1} u_k u_m \bar{u}_\ell \bar{u}_j + \mathcal{O}(\tau)$$

Aliasing problems and resonances.
Classical splitting : $\Omega_{km\ell j}(\tau) = \tau(|k|^2 + |m|^2 - |\ell|^2 - |j|^2)$.

Numerical experiments

$$i\partial_t u = -\Delta u + V \star u + |u|^2 u, \quad x \in \mathbb{T}^1.$$

$\hat{V}(k) = -\frac{2}{10+2k^2}$. Linear frequencies of the operator $H_0 = -\Delta + V\star$:

$$\omega_k = k^2 - \frac{2}{10 + 2k^2}, \quad k \in \mathbb{Z}.$$

Initial value :

$$u^0 = \frac{0.1}{4 - 2\cos(x)}$$

We use a collocation space discretization with $K = 400$ Fourier coefficients.

Numerical experiment : Standard splitting

Plot : Fourier coefficients $|\widehat{u}_k|^2$ in logarithmic scale. Splitting algorithm.

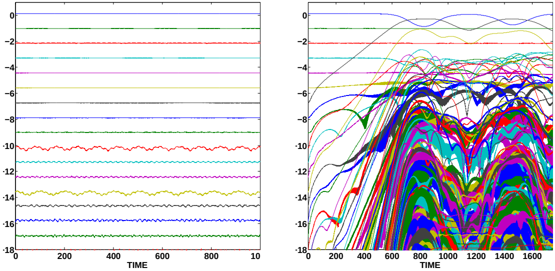


FIGURE – Right : $\tau = \dfrac{2\pi}{\omega_7 - \omega_1} \simeq 0.17459\ldots$, Left : $\tau = 0.174$

Implicit-explicit integrator

$$i\partial_t u = -\Delta u + V \star u + |u|^2 u, \quad x \in \mathbb{T}^1.$$

$$u^{n+1} = R(-i\tau H_0) \circ \varphi_P^\tau(u^n), \quad \text{with} \quad \left| \begin{array}{l} R(z) = \dfrac{1 + z/2}{1 - z/2}, \\ \varphi_P^\tau(u)(x) = e^{-i\tau|u(x)|^2} u(x) \end{array} \right.$$

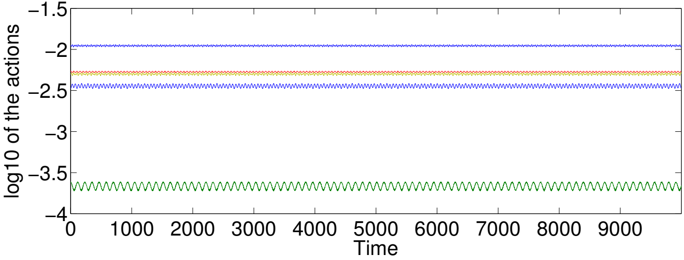
We consider as initial value the function

$$u^0 = \frac{0.1}{4 - 2\cos(x)} + 0.05(2e^{2ix} - 2e^{5ix} + 3e^{7ix}).$$

Collocation space discretization with $K = 200$ Fourier modes.

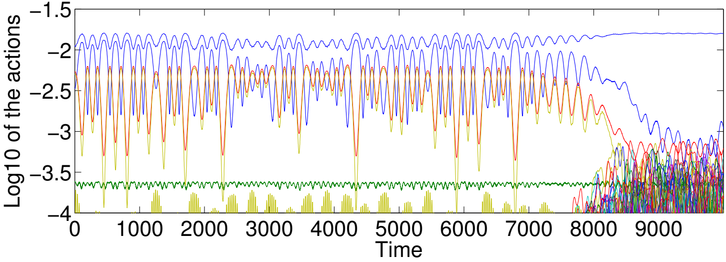
Implicit-explicit integrator

Evolution of the sum of the numerical actions $|\hat{u}_k^n|^2$ in logarithmic scale.



Stepsize $\tau = 0.13$. Long-time behavior as expected.

Implicit-explicit integrator



Stepsize $\tau = 0.1278\ldots$ such that

$$\arctan(\tau\omega_2/2) + \arctan(\tau\omega_5/2) - \arctan(\tau\omega_{-7}/2) = 0$$

Cancellation of the small divisor

$$\exp(2i\arctan(\tau\omega_2/2) + 2i\arctan(\tau\omega_5/2) - 2i\arctan(\tau\omega_{-7}/2)) - 1$$

Midpoint rule

$$i\partial_t u = -\Delta u + V \star u + |u|^2 u, \quad x \in \mathbb{T}^1.$$

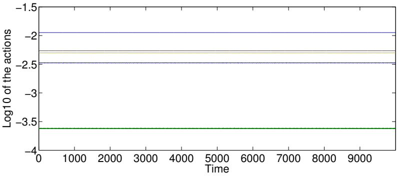
$$u^{n+1} = u^n - i\tau H_0\Big(\frac{u^{n+1}+u^n}{2}\Big) - i\tau g\Big(\frac{u^{n+1}+u^n}{2}\Big)$$

$g(u) = |u|^2 u.$

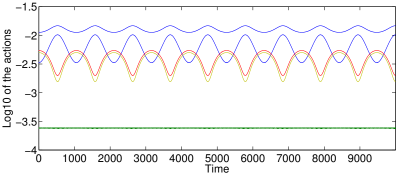
$$u^{n+1} = R(-i\tau H_0) \circ \Big(u^n - \frac{2i\tau}{2 - i\tau H_0} g\Big(\frac{u^{n+1}+u^n}{2}\Big)\Big).$$

Remark : can be interpreted as a splitting schemes !
Same parameters as before

Numerical experiment



Non-resonant step size.



Resonant step size with the arctan

Physical resonances.

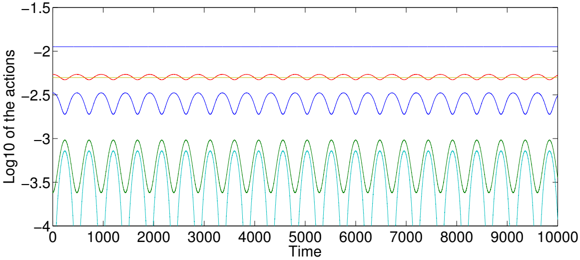
Same problem, but we construct a resonant situation :

$$\omega_2 = 10, \quad \omega_5 = 30 \quad \text{and} \quad \omega_{-7} = 40,$$

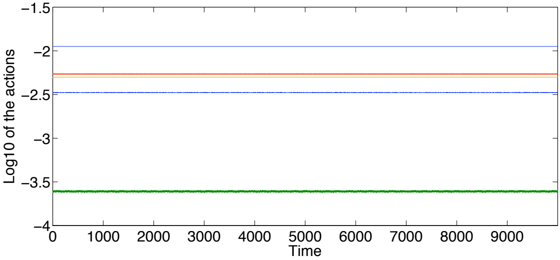
so that the ("physical") resonance relation holds :

$$\omega_2 + \omega_5 - \omega_{-7} = 0.$$

Exact solution : energy exchanges (Splitting scheme, CFL = 1)



Breaking physical resonances



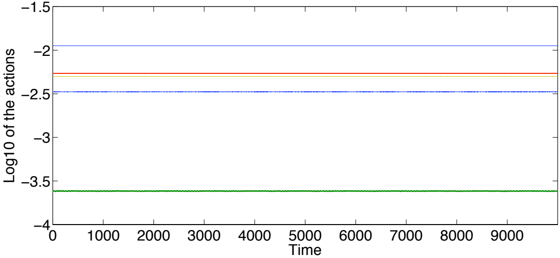
Implicit-explicit integrator with $\tau = 0.0812...$ such that

$$2\arctan(\tau\omega_2/2) + 2\arctan(\tau\omega_5/2) - 2\arctan(\tau\omega_{-7}/2) = \frac{1}{2}.$$

$$|\exp(2i\arctan(\tau\omega_2/2) + 2i\arctan(\tau\omega_5/2) - 2i\arctan(\tau\omega_{-7}/2)) - 1| \simeq 0.485...$$

but $\omega_2 + \omega_5 - \omega_7 = 0$! !

Breaking physical resonances



Undesired actions preservation by the midpoint rule.

Energy cascades

NLS on the two-dimensional torus

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u, \quad x \in \mathbb{T}^2,$$

and we take as initial data

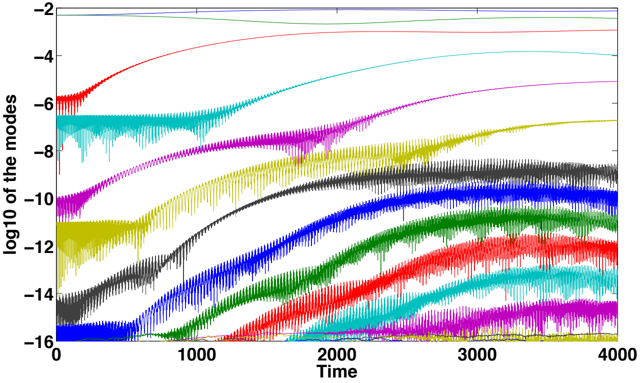
$$u(0,x) = 1 + 2\cos(x_1) + 2\cos(x_2).$$

There exists energy cascaces (Carles & Faou, 2012).
Resonant modulus

$$\begin{cases} |a|^2 + |b|^2 - |c|^2 - |d|^2 = 0 \\ a + b - c - d = 0 \in \mathbb{Z}^2 \end{cases} \Longrightarrow (a, c, b, d) \quad \text{rectangle.}$$

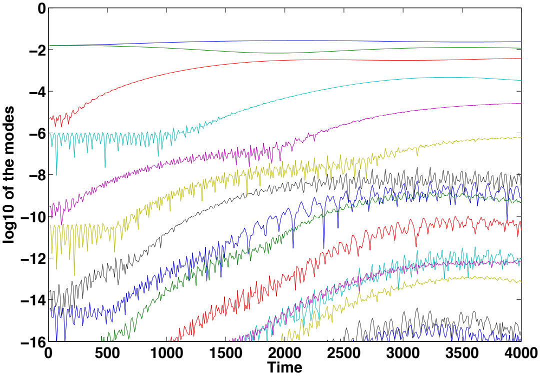
Energy cascade

Numerical reproduction of these energy exchanges is not guaranteed in general. Explicit scheme, CFL = 0.1



Energy cascade

Explicit scheme, $\tau = 0.1$, grid 128×128.



Midpoint barrage

Implicit explicit integrators : No energy cascade.