Existence and stability of solitons for fully discrete approximations of the nonlinear Schrödinger equation

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Solitons

NLS on the real line :

$$i\psi_t = -\psi_{xx} - |\psi|^2\psi, \quad x \in \mathbb{R}, \ t \in \mathbb{R}.$$

Hamiltonian and L^2 norm

$$H(\psi) := \int_{\mathbb{R}} \left[|\psi_x|^2 - \frac{|\psi|^4}{2} \right] \mathrm{d}x, \quad \text{and} \quad N(\psi) := \int_{\mathbb{R}} |\psi|^2 \, \mathrm{d}x.$$

Gauge invariance $\psi \mapsto e^{i\alpha}\psi$. Particular solution

$$\psi(t,x) = e^{i\lambda t}\eta(x) \quad \text{with} \quad \eta(x) := \frac{1}{\sqrt{2}} \mathrm{sech}\left(\frac{x}{2}\right),$$

η solves the variational problem $\min\limits_{N(\psi)=1} H(\psi)$

Orbital stability

Orbit of the soliton

$$\Gamma = \bigcup_{\alpha} e^{i\alpha t}\eta(x)$$

For symmetric perturbation ($\psi(x) = \psi(-x)$) then

$$\mathrm{dist}(\psi(0), \Gamma) < \delta \quad \Longrightarrow \quad \mathrm{dist}(\psi(t), \Gamma) < C\delta, \quad t \in \mathbb{R}.$$

Distance measured in H^1.
Weinstein (84), Grillakis, Shatah and Strauss (87)

- Can we reproduce this numerically ?
  Important benchmark in numerical analysis since 30 years.
- Numerical simulation : space and time discretization

Discretization : Level 1 (space)

$\psi_\ell \simeq \psi(h\ell)$, $\ell \in \mathbb{Z}$. Discrete nonlinear Schrödinger equation (DNLS) :

$$i\dot{\psi}_\ell = -\frac{1}{h^2}(\psi_{\ell+1} + \psi_{\ell-1} - 2\psi_\ell) - |\psi_\ell|^2\psi_\ell, \quad \ell \in \mathbb{Z} \,.$$

Discrete Hamiltonian function and L^2 norm given by

$$H_h(\psi) = h\sum_{j\in\mathbb{Z}}\left[\left|\frac{\psi_j - \psi_{j-1}}{h}\right|^2 - \frac{|\psi_j|^4}{2}\right] \quad \text{and} \quad N_h(\psi) = h\sum_{j\in\mathbb{Z}}|\psi_j|^2.$$

The discrete space of functions is

$$V_h = \{\psi_j \in \mathbb{C}^{\mathbb{Z}} \,|\, \psi_j = \psi_{-j}\}$$

equipped with the discrete norm

$$\|\psi\|_h^2 = 2h\sum_{j\in\mathbb{Z}}\frac{|\psi_{j+1} - \psi_j|^2}{h^2} + h\sum_{j\in\mathbb{Z}}|\psi_j|^2.$$

Discretization : Level 1 (Finite differences)

Finite elements : $s : \mathbb{R} \to \mathbb{R}$

$$s(x) = \begin{cases} 0 & \text{if} \quad |x| > 1, \\ x + 1 & \text{if} \quad -1 \leq x \leq 0, \\ -x + 1 & \text{if} \quad 0 \leq x \leq 1, \end{cases}$$

Embedding $i_h : V_h \to H^1(\mathbb{R}; \mathbb{C})$ defined by

$$\{\psi_j\}_{j \in \mathbb{Z}} \mapsto (i_h \psi)(x) := \sum_{j \in \mathbb{Z}} \psi_j s\left(\frac{x}{h} - j\right) \ .$$

Important property :

$$H(i_h \psi) - H_h(\psi) = \mathcal{O}(h \|\psi\|_h^2)$$

Bambusi & Penati (2010) : existence of discrete ground state for DNLS.

Discretization : Level 2 (Dirichlet cut-off)

Large number $K \geq 1$:

$$\begin{cases} i\dot{\psi}_\ell = -\frac{1}{h^2}(\psi_{\ell+1} + \psi_{\ell-1} - 2\psi_\ell) - |\psi_\ell|^2\psi_\ell, & -K \leq \ell \leq K \\ \psi_{\pm(K+1)} = 0. \end{cases}$$

Finite dimensional space

$$V_{h,K} := \{(\psi_j)_{j\in\mathbb{Z}} \in V_h \,|\, \psi_j = 0 \quad \text{for} \quad |j| \geq K+1\}$$

Discrete energies and norms

$$H_{h,K} := H_h|_{V_{h,K}} \quad \text{and} \quad N_{h,K} := N_h|_{V_{h,K}}$$

Embedding in H^1 : $i_{h,K} = i_h|_{V_{h,K}}$.

Discretization : Level 3 (Time splitting integrator)

ψ^n approximation of $\psi(t)$ at time $n\tau$: Symplectic splitting

$$\psi^{n+1} = \Phi_A^\tau \circ \Phi_P^\tau(\psi^n),$$

- Flow Φ_P^τ is the exact solution of

$$i\dot{\psi}_\ell = -|\psi_\ell|^2\psi_\ell, \quad \ell = -K, \ldots, K\,,$$

  $\Phi_P^\tau(\psi)_\ell = \exp(i\tau|\psi_\ell|^2)\psi_\ell.$

- Flow Φ_A^τ, solution of

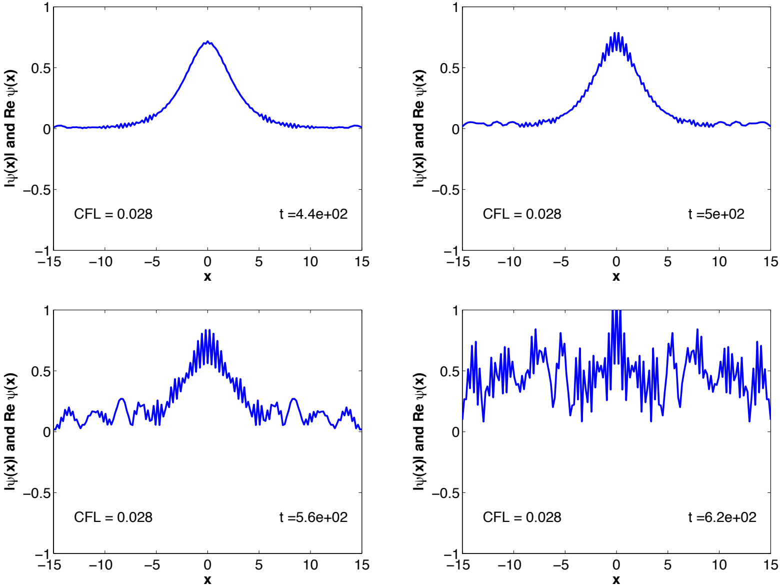
$$i\dot{\psi}_\ell = -\frac{1}{h^2}(\psi_{\ell+1} + \psi_{\ell-1} - 2\psi_\ell), \quad \ell = -K, \ldots, K \;\; ,$$

  Exponential of a tridiagonal matrix.

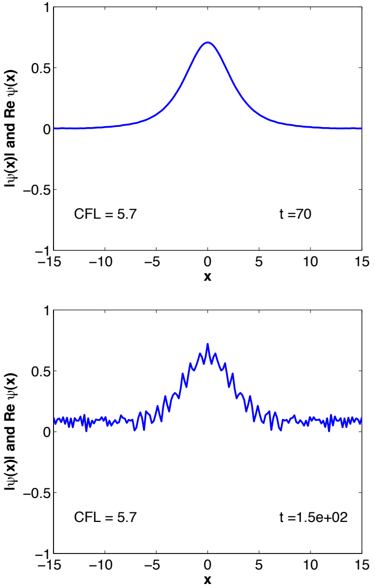
$$\text{Courant-Friedrich-Lewy number} \quad CFL = \frac{\tau}{h^2}$$

Geometric nature of the integrator is very important.

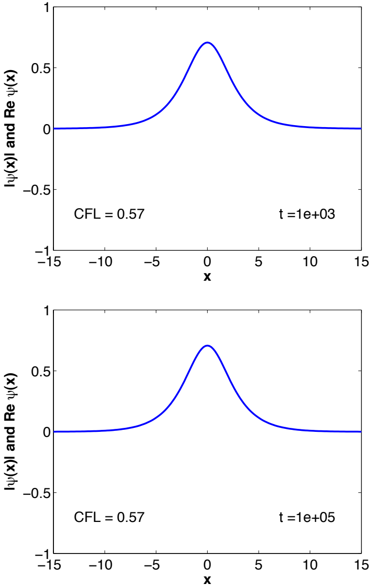
$CFL = 0.028$. Non symplectic scheme.



Symplectic splitting. $h = 0.1875$, $K = 80$, $\tau = 0.2$, $CFL = 5.7$.

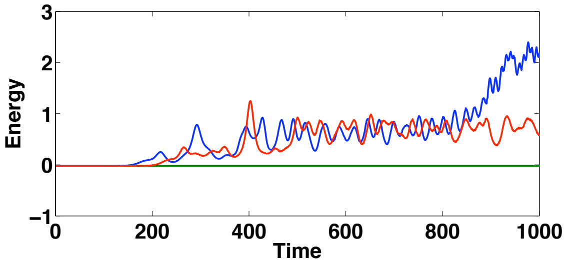


Symplectic splitting : CFL 0.57.



Evolution of the energy

$$H_h(\psi) = h \sum_{j \in \mathbb{Z}} \left[\left| \frac{\psi_j - \psi_{j-1}}{h} \right|^2 - \frac{|\psi_j|^4}{2} \right]$$



- CFL = 19.8 : Energy drift
- CFL = 9.9 : Energy drift
- CFL = 1.9 : No drift.

Main result

Theorem

CFL condition

$$(2M+3)\frac{\tau}{h^2} < \frac{2\pi}{3},$$

then if $(\psi_j^0)_{j=-K}^{K} \in V_{h,K}$ *is such that*

$$\mathrm{dist}(i_{h,K}\psi^0, \Gamma) \leq \delta,$$

then

$$\forall\, n\tau \leq \tau^{-M}, \quad \mathrm{dist}(i_{h,K}(\Phi_A^\tau \circ \Phi_P^\tau)^n \psi^0, \Gamma) \leq C_2\Big(\delta + h + \frac{\tau}{h} + \frac{1}{h^2} e^{-C_1 K h}\Big).$$

RHS sufficiently small, C_1, C_2 independent of τ, h and K.

Orbital stability : the continuous case

V space of H^1 symmetric functions. Local coordinate system around Γ :

$$\mathbb{T} \times \mathbb{R} \times W \ni (\alpha, r, u) \mapsto \chi(\alpha, r, u) = e^{i\alpha}((1+r)\eta + u) \in V,$$

with $W = \{ u \in V | \langle u, \eta \rangle = \langle u, i\eta \rangle = 0\}$ and $\langle \varphi, \psi \rangle = \mathrm{Re} \int_{\mathbb{R}} \varphi \overline{\psi}$.

- Locally well defined and invertible around Γ
- $r(u)$ defined by $N(\chi(\alpha, r(u), u)) = 1$.
- $\mathcal{H}(u) := H(\chi(\alpha, r(u), u)$. Then

$$\mathrm{d}\mathcal{H}(0) = 0, \quad \text{and} \quad \forall\, U \in W, \quad \mathrm{d}^2\mathcal{H}(0)(U, U) \geq c \|U\|_{H^1}^2 .$$

$$|H(\psi) - H(\eta)| = |\mathcal{H}(u) - \mathcal{H}(0)| \geq c\|u\|_{H^1}^2 \geq c\,\mathrm{dist}(\psi, \Gamma)^2.$$

- Conclusion using the preservation of the energy.

Orbital stability : the discrete case

Set of parameter $\Sigma \in \mathbb{R}^p$, $\epsilon : \Sigma \to \mathbb{R}^+$.
For $\mu \in \Sigma$, Hilbert space $(V_\mu, \|\cdot\|_\mu)$ satisfying

(i) $\exists\, i_\mu : V_\mu \to H^1$ and a projection $\pi_\mu : H^1 \mapsto V_\mu$ gauge invariant and

$$\left| \|\varphi_\mu\|_\mu^2 - \|i_\mu \varphi_\mu\|_{H^1}^2 \right| \leq \epsilon(\mu) \|i_\mu \varphi_\mu\|_{H^1}^2 .$$

(ii) $\exists\, N_\mu(\psi_\mu) = \langle \psi_\mu, \psi_\mu \rangle_\mu$ modified L^2 norm

$$\|N \circ i_\mu - N_\mu\|_{\mathcal{C}^2(B_\mu(R_0))} \leq \epsilon(\mu).$$

(iii) $\exists\, H_\mu : V_\mu \to \mathbb{R}$ which is a modified Hamiltonian

$$\|H \circ i_\mu - H_\mu\|_{\mathcal{C}^2(B_\mu(R_0))} \leq \epsilon(\mu).$$

(iv) If η is the continuous ground state we have

$$\|i_\mu \pi_\mu \eta - \eta\|_{H^1} \leq \epsilon(\mu).$$

Orbital stability : the discrete case

Theorem

For all $\mu \in \Sigma$ *with* $\epsilon(\mu) < \epsilon_0$, $\exists\, \eta_\mu \in V_\mu$ *that realizes the minimum of* H_μ *under the constraint* $N_\mu(\psi_\mu) = 1$. *Moreover,*

$$\|\eta_\mu - \pi_\mu \eta\|_{V_\mu} \leq \epsilon(\mu).$$

and

$$\mathrm{dist}(i_\mu \psi_\mu, \Gamma)^2 \leq C(|H_\mu(\psi_\mu) - H_\mu(\eta_\mu)| + \epsilon(\mu)),$$

for all ψ_μ *such that* $\mathrm{dist}(i_\mu \psi_\mu, \Gamma) \leq \gamma_0$ *and* $N_\mu(\psi_\mu) = 1$.

Sketch of proof

Local coordinate system around $\pi_\mu \Gamma$:

$$\mathbb{T} \times \mathbb{R} \times W_\mu \ni (\alpha, r, u_\mu) \mapsto \chi(\alpha, r, u_\mu) = e^{i\alpha}((1+r)\pi_\mu \eta + u_\mu) \in V_\mu,$$

with $W_\mu = \{\ u_\mu \in V_\mu | \langle u, \pi_\mu \eta \rangle_\mu = \langle u, i\pi_\mu \eta \rangle_\mu = 0\}$.

- Locally well defined and invertible around $\pi_\mu \Gamma$ uniformly in μ
- $r_\mu(u_\mu)$ defined by $N_\mu(\chi(\alpha, r_\mu(u_\mu), u_\mu)) = 1$.
- $\mathcal{H}_\mu(u) := H(\chi(\alpha, r_\mu(u_\mu), u_\mu)$. Then

$$\|\mathcal{H} \circ i_\mu - \mathcal{H}_\mu\|_{\mathcal{C}^2(B_\mu(R_0))} \leq \epsilon(\mu).$$

  Implies that $\mathcal{H}_\mu$ is convex and has a unique minimum.

Orbital stability : the discrete case

Level 1 (space discretization)

$$\Sigma = \{ h \in \mathbb{R} \}, \quad \text{and} \quad \epsilon(\mu) = h.$$

$$|H(i_h\psi) - H_h(\psi)| + |N(i_h\psi) - N_h(\psi)| = \mathcal{O}(h\|\psi\|_h^2)$$

Projection : $(\pi_h u)_\ell = u(\ell h)$ then

$$\|i_h \pi_h u - u\|_{H^1} \leq h\|u\|_{H^2}$$

As the flow of DNLS preserve the energy H_h, we have

$$\mathrm{dist}(i_h\psi_h(t), \Gamma) \leq \delta \quad \Longrightarrow \forall\, t \in \mathbb{R}, \quad \mathrm{dist}(i_h\psi_h, \Gamma) \leq C(\delta + h).$$

Orbital stability : the discrete case

Level 1 + 2 (space discretization + Dirichlet cut-off)

$$\Sigma = \{ (h, K) \in \mathbb{R} \times \mathbb{N} \}$$

Control of the energy and L^2 as before

$$\begin{aligned}
\|i_{h,K}\pi_{h,K}\eta - \eta\|_{H^1} &\leq C\|i_{h,K}\pi_{h,K}\eta - i_{h,K}\pi_h\eta\|_{H^1} + \|i_h\pi_h\eta - \eta\|_{H^1} \\
&\leq C(\|\pi_{h,K}\eta - \pi_h\eta\|_{V_h} + h) \\
&\leq C(h + \frac{1}{h^2}e^{-C_1 Kh})
\end{aligned}$$

As the flow of DNLS + Dirichlet preserves the energy H_h, we have

$$\mathrm{dist}(i_{h,K}\psi_{h,K}(t), \Gamma) \leq \delta \quad \Longrightarrow \forall\, t \in \mathbb{R},$$

$$\mathrm{dist}(i_{h,K}\psi_{h,K}, \Gamma) \leq C(\delta + h + \frac{1}{h^2}e^{-C_1 Kh}).$$

Orbital stability : the discrete case

Level 1 + 2 + 3 (space discretization + Dirichlet cut-off + Splitting)

$$\Sigma = \{ (h, K, \tau) \in \mathbb{R} \times \mathbb{N} \times \mathbb{R} \}$$

Main problem : What is the modified energy ? ?

Orbital stability : the discrete case

Level 1 + 2 + 3 (space discretization + Dirichlet cut-off + Splitting)

$$\Sigma = \{ (h, K, \tau) \in \mathbb{R} \times \mathbb{N} \times \mathbb{R} \}$$

Main problem : What is the modified energy ? ?

Theorem (Hamiltonian interpolation)

$M \in \mathbb{N}$ be fixed. CFL condition $(2M+3)\frac{\tau}{h^2} < \frac{2\pi}{3}$. For all $\mu = (h, K, \tau) \in \Sigma$,
$\exists H_\mu$ defined on V_μ such that

$$\|H_\mu - H \circ i_\mu\|_{C^2(B_\mu(R_0))} \leq C\frac{\tau}{h}$$

and for all $\psi \in V_\mu$ with $\|\psi\|_\mu \leq R_0$,

$$\|\Phi_P^\tau \circ \Phi_A^\tau(\psi) - \Phi_{H_\mu}^\tau(\psi)\|_\mu \leq C\tau^{M+1}$$

Hamiltonian interpolation : principles

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

Baker-Campbell-Haussdorf formula

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

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

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

Hamiltonian interpolation : principles

Nonlinear Hamiltonian systems $\dot{y} = J^{-1}\nabla H(y)$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

- $H = H_1 + H_2$. Numerical method : $\Phi^\tau = \phi^\tau_{H_1} \circ \phi^\tau_{H_2}$.
- In this situation

$$\begin{aligned} \Phi^\tau &= \exp(\tau \mathcal{L}_{H_1}) \circ \exp(\tau \mathcal{L}_{H_2}) \\ &= \exp(\tau \mathcal{L}_{H_\tau}) + \text{very small} \end{aligned}$$

  with $H_\tau = H_1 + H_2 + \frac{1}{2}\tau\{H_1, H_2\} + \cdots$
- Analytic estimates : After a truncation at the order N, we have

$$\text{very small} = (C\tau N)^N \quad \text{over a compact} \quad K$$

Hamiltonian interpolation

Theorem (Benettin & Giorgilli 1994)

Let Φ^τ be a symplectic integrator of order p, and $y^{n+1} = \Phi^\tau(y^n)$, $n \geq 0$. Assume $\{y^n\}_{n\in\mathbb{N}}$ bounded and H analytic. Then there exists

$$\tilde{H}_\tau(y) = H(y) + \mathcal{O}(\tau^p)$$

such that

$$\|\phi^\tau_{\tilde{H}_\tau}(y) - \Phi^\tau(y)\| \leq \exp(-1/c\tau)$$

Consequence :

$$\forall\, n\tau \leq \exp(1/c\tau) \quad , \quad |H(y^n) - H(y^0)| \; \leq C\tau^p.$$

Fundamental result in *Geomeric integration*.

Hamiltonian interpolation : principles

$$\partial_t u = iAu + iBu$$

- Problem : $A = -\Delta$ is not bounded.
- Linear case : the BCH does not converge
- Nonlinear case : estimate in a Banach space under assumptions on a much smaller space.

$$\|\phi^\tau_{H_1} \circ \phi^\tau_{H_2}(y) - \phi^\tau_{H_\tau}(y)\|_{L_2} = \mathcal{O}(\tau^N C(\|y\|_{H^{2N}})).$$

A priori bound of the numerical solution in all the H^s.
Prevents a fair use of the bootstrap argument.

Hamiltonian interpolation : principles

Find $Z(t)$ such that

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

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 : $Z(t) = \tau A + tZ_1 + \cdots$
- Second term :

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

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

Hamiltonian interpolation : principles

The modified energy is well defined if $\|\mathrm{ad}_{\tau A}\| < 2\pi$. Example in the linear case

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

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

$$\big(\mathrm{ad}_{\tau A} W\big)_{k\ell} = \tau(|k|^2 - |\ell|^2)W_{k\ell}.$$

- $(Z_1)_{k\ell} = \widehat{V}_{k-\ell}\frac{i\tau(|k|^2-|\ell|^2)}{\exp(i\tau(|k|^2-|\ell|^2)-1}$ well defined for $\tau(|k|^2 - |\ell|^2) < 2\pi$

Hamiltonian interpolation : principles

Nonlinear case :

$$(\tau A\psi)_\ell = \tau \frac{\psi_{\ell+1} + \psi_{\ell-1} - 2\psi_\ell}{\mu^2},$$

then if P is a polynomial of degreee r,

$$\|\mathrm{ad}_{\tau A} P\| \leq 3(r+1)\frac{\tau}{h^2}\|P\|$$

The CFL is more restrictive for constructing the term Z_m, $m \geq 1$.

Resonant time steps

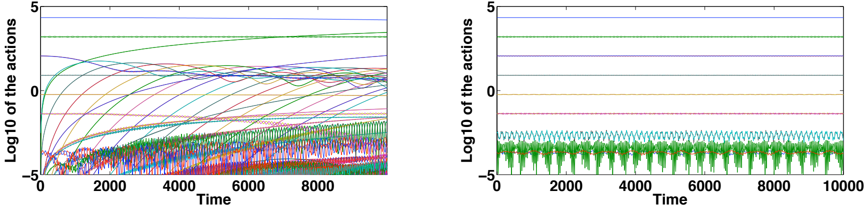
Back to the linear case : $\partial_t u = -i\Delta u + iVu, \quad x \in \mathbb{T}.$

- Splitting : $u^{n+1} = e^{-i\tau\Delta} \circ e^{i\tau V} u^n$.
- Existence of a modified energy :
  avoid small denominators $\tau(|k|^2 - |\ell|^2) \simeq 2k\pi$.
- What happens if we use a resonant time-step ?
- Example :

$$V(x) = 0.01 \frac{3}{5 - 4\sin(x)} \quad \text{and} \quad u^0(x) = \frac{2}{2 - \cos(x)}.$$

Plot of the evolution of the Fourier coefficients.

Resonant time steps



$$\tau = \frac{2\pi}{6^2 - 2^2} \simeq 0.1963\ldots \text{ (left)} \quad \text{and} \quad \tau = 0.2 \quad \text{(right)}.$$

Resonant time steps

Theorem

For all $q \in \mathbb{N}^*$, take $\tau = 2\pi/q$. Then there exists $V(x) \in H^s$, $s \geq 1$, uniformly bounded in q, such that for all $w(x) \in H^s$,

$$\lim_{n\to\infty} \left\|(e^{-i\tau\Delta} \circ e^{i\tau V})^n w(x)\right\|_{H^s} = +\infty.$$

Proof : Take $V = c_q W(qx)$, normalized in H^s,

$$\begin{aligned}([e^{-i\tau\Delta}, V])_{k\ell} &= \hat{V}_{k-\ell}(e^{i\tau k^2} - e^{i\tau \ell^2}) \\ &= e^{i\tau\ell^2}\hat{V}_{k-\ell}(e^{i\tau(k^2-\ell^2)} - 1) = 0\end{aligned}$$

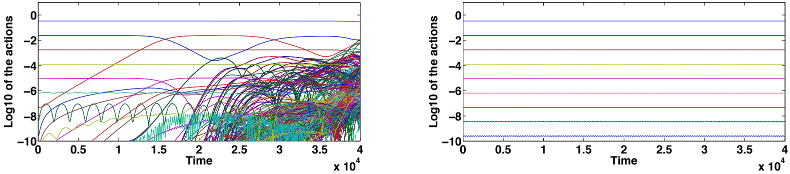
because $\widehat{V}_{k-\ell} \neq 0$ only if $q \,|\, k - \ell$ for which $\tau(k^2 - \ell^2) = 2\pi k$.
In other words

$$(e^{-i\tau\Delta} \circ e^{i\tau V})^n w(x) = e^{-in\tau\Delta} \circ e^{in\tau V} w(x)$$

and $\left\|e^{in\tau V} w(x)\right\|_{H^s} \to +\infty$ when $n \to \infty$.

Resonant time steps

Non-linear case : $\partial_t u = -i\Delta u + i|u|^2 u, \quad x \in \mathbb{T}.$
Splitting : $u^{n+1} = e^{-i\tau\Delta} \circ \varphi_P^\tau(u^n)$. $u^0(x) = \frac{0.1}{2-\cos(x)}$



with the stepsize

$$\tau = \frac{2\pi}{12^2 - 5^2 - 7^2} \simeq 0.0898\ldots \quad \text{and} \quad \tau = 0.9$$

Resonant time steps

Theorem

For all $q \in \mathbb{N}^*$, take $\tau = 2\pi/q$. Then there exists $u^0(x) \in H^s$, $s \geq 1$, uniformly bounded in q, such

$$\lim_{n\to\infty} \|(e^{-i\tau\Delta} \circ \varphi_P^\tau)^n u^0(x)\|_{H^s} = +\infty.$$

Proof : $\varphi_P^t(u^0) = e^{it|u^0(x)|}u^0(x)$.

$u^0(x) = U(qx) \Longrightarrow \varphi_P^t(u^0) = F(qx)$.

But $e^{-i\tau\Delta}F(qx) = F(qx)$ for $\tau = 2\pi/q$.

So $\|(e^{-i\tau\Delta} \circ \varphi_P^\tau)^n U(qx)\|_{H^s} = \|\varphi_P^{n\tau} U(qx)\|_{H^s} \to \infty$ when $n \to \infty$.

More "generic" result using resonant normal forms
(work in progress with B. Grébert).