Backward error analysis for Hamiltonian PDEs

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A first example

Focusing Schrödinger equation on $\mathbb{R}$

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

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

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

- Splitting schemes : For small τ,

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

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 $[-\pi/L, \pi/L]$ (L small). Fourier pseudo spectral methods with K equidistant points.
- First case : Splitting method.

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

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

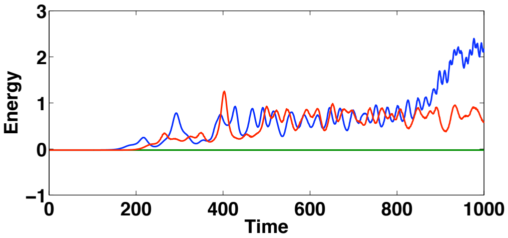
$$\text{cfl} = \tau L^2 \left(\frac{K}{2}\right)^2.$$

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

Solitary waves

Evolution of the energy

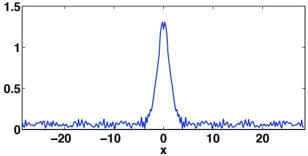
$$H(u,\bar{u}) = \int_{\mathbb{R}} |\partial_x u(x)|^2 - \frac{1}{2}|u(x)|^4 \mathrm{d}x$$

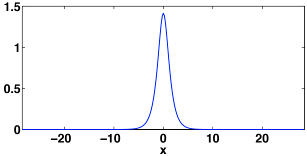


- $\tau = 0.1$ (cfl $= 19.8$) : Energy drift
- $\tau = 0.05$ (cfl $= 9.9$) : Energy drift
- $\tau = 0.01$ (cfl $= 1.9$) : No drift.

Solitary waves

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

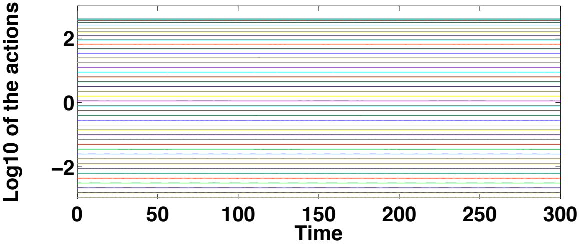




- cfl $= 19.8$ at time $t = 300$ (left)
- cfl $= 1.9$ at time $t = 10000$ (right)

Solitary waves

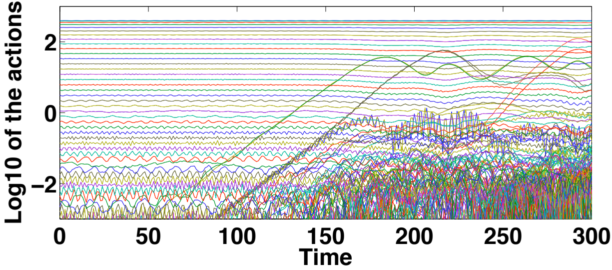
Plot of the Fourier coefficients $|\hat{u}_k(t)|^2$ for $k \in \mathbb{Z}$ in log scale.



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

Same computation with the implicit-explicit integrator :

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

with

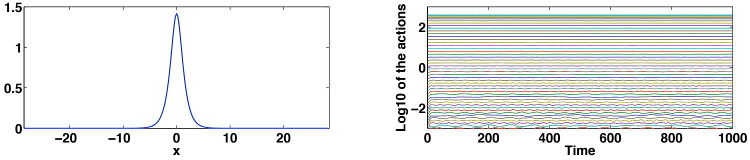
$$R(i\tau\Delta) = \frac{1 + i\tau\Delta/2}{1 - i\tau\Delta/2}$$

Midpoint rule applied to the free Schrödinger equation

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

We use cfl $= 19.8$.

Solitary waves



No energy drift, preservation of the regularity, even with cfl $= 19.8$.

How to explain this ?

Convergence of splitting methods

NLS on the d-dimensional torus with polynomial nonlinearity .

$$i\partial_t u = \Delta u + \partial_{\bar{u}} P(u, \bar{u}) \qquad (H = T + P)$$

- Wiener algebra :

$$u = \sum_{\in \mathbb{Z}^d} \hat{u}_k e^{ikx} \qquad \|u\|_{\ell^1_s} := \sum_{k \in \mathbb{Z}^d} |k|^s |\hat{u}_k|.$$

- Fully discrete solution ($\mathcal{F}_K$ Discrete Fourier transform)

$$u^{K,n+1} = \mathcal{F}_K^{-1} \circ \phi_T^\tau \circ \mathcal{F}_K \circ \phi_P^\tau (u^{K,n})$$

Theorem

$s \geq 2$. If $u(t) \in \ell^1_{s+2}$ for $t \in (0, t_*)$. $\ell^1 = \ell^1_0$

$$\|u(n\tau) - u^{K,n+1}\|_{\ell^1} \leq C(\tau + K^{-s}).$$

Finite dimensional situation

Hamiltonian ODE : $H : \mathbb{R}^d \to \mathbb{R}$,

$$\dot{y} = X_H(y) := J^{-1}\nabla H(y), \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

- $\mathcal{L}_H$ the Lie derivative :

$$\begin{aligned} \mathcal{L}_H G &= \frac{\mathrm{d}}{\mathrm{d}t} G \circ \phi_H^t(y) = (\nabla H)^T J \nabla G \\ &=: \{H, G\} \end{aligned}$$

- Exact flow : $\phi_H^t(y) = \exp(t\mathcal{L}_H)[Id](y) = y + tX_H(y) + \cdots$
- Numerical approximation :

$$\Phi^\tau(y) = y + \tau X_H(y) + \cdots$$

- BEA problem : Can we "take the Log", and write

$$\Phi^\tau(y) = \exp(\tau \mathcal{L}_{H_\tau})[Id](y) + \text{very small}.$$

Finite dimensional situation

Hypothesis :

- Φ^τ symplectic method (Midpoint, splitting,...)
- The numerical trajectory remains bounded : for all τ,

$$y_{n+1} = \Phi^\tau(y_n), \qquad \{y_n \,|\, n \in \mathbb{N}\} \subset K$$

- H analytic (over K).

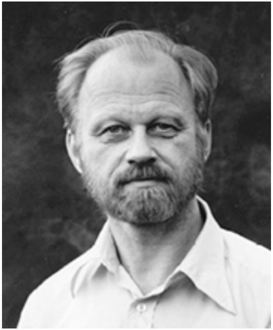
Then there exists $H_\tau = H + \tau H_1 + \tau^2 H_2 + \cdots$,

$$\Phi^\tau(y) = \exp(\tau \mathcal{L}_{H_\tau})[Id](y) + \mathcal{O}(\exp(-1/(c\tau)))$$

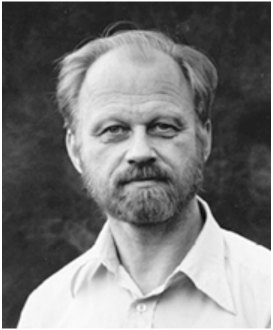
Benettin & Giorgilli [94], Hairer & Lubich [97], Reich [99], ...

- c : eigenvalues of $\nabla^2 H$ over K.
- Corollary : H_τ (and hence H) is preserved over exponentially long time, KAM, stability, etc...

Origin : Hamiltonian interpolation



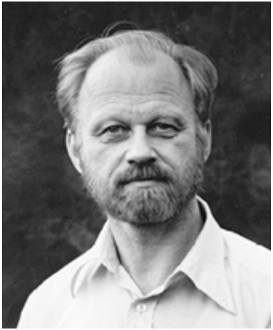
Origin : Hamiltonian interpolation



Jürgen Moser (Königsberg 1928, Zürich 1999)

1968 : A discrete sympletic map close to the identity can be interpolated by a Hamiltonian flow

Origin : Hamiltonian interpolation



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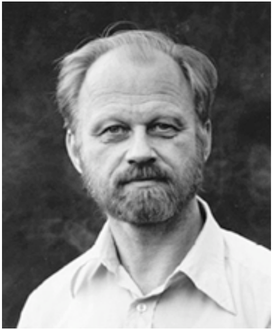

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1968 : A discrete sympletic map close to the identity can be interpolated by a Hamiltonian flow
1994-99 : Application to symplectic integrators for ODEs
Today : Try to apply Moser's idea to Hamiltonian PDEs

The case of splitting methods

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

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

  and we take $N = 1/(C\tau e)$.

Problem in infinite dimension

- $H = H_1 + H_2$. NLS : $H_1 = -\Delta$ and $H_2 = |u|^2 u$.
- In this situation

$$\begin{aligned} \Phi^\tau &= \exp(\tau \mathcal{L}_{H_1}) \circ \exp(\tau \mathcal{L}_{H_2}) \\ &= \exp(\tau \mathcal{L}_{H_\tau}) + \text{defect in } L^2 \end{aligned}$$

After truncation at the order N :

$$(\text{defect in } L^2) = \tau^N C_N(\|y\|_{H^N})$$

- Hypothesis : y_n remains bounded in all the H^s and all time ? ? not fair and false in general (resonances, CFL required, etc...).

Linear Schrödinger equation

- Consider the linear Schrödinger equation on the torus

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

- $x \in \mathbb{T}^d$. $\Delta = \sum_{j=1}^d \partial_{x_j}^2$.
- $V(x) \in \mathbb{R}$ potential function.
- Conservation of the L^2 norm and of the energy

$$H(u) = \frac{1}{2}\int_{\mathbb{T}^d} \Big[|\nabla u(x)|^2 + V(x)u(x)^2\Big]\mathrm{d}x.$$

- Exact solution : $u(t) = \exp(it(-\Delta + V))u_0$.

Splitting schemes

- Standard splitting

$$u^{n+1} = \exp(-i\tau\Delta)\exp(i\tau V)u^n$$

- Order 1 scheme (Jahnke & Lubich, 2000) if u^n remains smooth.
- Mid-split scheme :

$$u^{n+1} = R(-i\tau\Delta)\exp(i\tau V)u^n$$

where

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

Implicit-explicit integrators

- We have
$$\frac{1+ix}{1-ix} = \exp(2i\arctan(x)).$$

$$R(-i\tau\Delta) = \frac{1-i\tau\Delta/2}{1+i\tau\Delta/2} = \exp(2i\arctan(-\tau\Delta/2)) =: \exp(iA_0).$$

- New approach : find $Z(t)$ such that for a fixed τ,
$$\forall t \leq \tau, \quad \exp(itV)\exp(iA_0) = \exp(iZ(t))$$
  and then make $t = \tau$.
- First remark : $Z(0) = A_0$ depends on τ.
- Taking the derivative in t yields
$$iV\exp(itV)\exp(iA_0) = i\left(\mathrm{d}\exp_{iZ(t)} Z'(t)\right)$$

Implicit-explicit integrators

- $Z(t)$ has to satisfy the equation

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

- $\mathrm{ad}_A(B) = [A, B] = AB - BA.$
- B_n Bernoulli numbers. $\displaystyle\sum_{n=0}^{\infty} \frac{B_n}{n!} x^n = \frac{x}{e^x - 1}.$
- Expansion :

$$Z(t) = A_0 + tZ_1 + \cdots$$

then

$$A_0 = -2 \arctan\left(\frac{\tau\Delta}{2}\right)$$

In Fourier : Diagonal operator with coefficients

$$(A_0)_{kk} = 2 \arctan\left(\frac{\tau|k|^2}{2}\right), \quad k \in \mathbb{Z}^d.$$

Implicit-explicit integrators

- Second term :

$$Z_1 = \sum_{n \geq 0} \frac{B_n}{n!} i^k \mathrm{ad}^n_{A_0}(V).$$

- $A = (A_{k\ell})_{k,\ell \in \mathbb{Z}^d}$ operator acting on Fourier coefficients

$$\left\|A\right\|_\alpha = \sup_{k,\ell} |A_{k\ell}| \big(1 + |k - \ell|^\alpha\big).$$

  We have

$$\left\|AB\right\|_\alpha \leq C_\alpha \left\|A\right\|_\alpha \left\|B\right\|_\alpha .$$

- Operator associated with V : $V_{k\ell} = \hat{V}_{k-\ell}$.
- $V \in H^s$ implies $\left\|V\right\|_s < \infty$.

Implicit-explicit integrators

Lemma

We have for $\alpha \geq 0$

$$\|\mathrm{ad}_{A_0} B\|_\alpha \leq \pi \|B\|_\alpha$$

Proof : A_0 is diagonal.

$$\begin{aligned}\left(\mathrm{ad}_{A_0} W\right)_{k\ell} &= \left((A_0)_{kk} - (A_0)_{\ell\ell}\right) W_{k\ell}, \\ &= \left(2\arctan(\tau|k|^2/2) - 2\arctan(\tau|\ell|^2/2)\right) W_{k\ell}.\end{aligned}$$

and

$$\left|2\arctan(\tau|k|^2/2) - 2\arctan(\tau|\ell|^2/2)\right| < \pi.$$

This lemma is false for the exact splitting without CFL

In this case $A_0 = \tau\Delta$ and

$$\left(\mathrm{ad}_{A_0} W\right)_{k\ell} = \tau(|k|^2 - |\ell|^2) W_{k\ell} \ldots$$

Implicit-explicit integrators

- Second term : Infinite series

$$Z_1 = \sum_{n \geq 0} \frac{B_n}{n!} i^k \mathrm{ad}^n_{A_0}(V).$$

- We have

$$\|Z_1\|_\alpha \leq \|V\|_\alpha \sum_{n \geq 0} \frac{|B_n|}{n!} \pi^n < \infty.$$

- Radius of convergence of the Bernoulli power series : 2π ! !
- In terms of coefficients

$$(Z_1)_{k\ell} = V_{k\ell} \frac{i(\lambda_k - \lambda_\ell)}{\exp(i(\lambda_k - \lambda_\ell)) - 1}$$

  - Mid-split integrators : $\lambda_k = 2 \arctan(\tau |k|^2 / 2)$.
  - Exact splitting with CFL : $\lambda_k = \tau |k|^2 \leq \pi$.

Control of the small divisors $\exp(i(\lambda_k - \lambda_\ell)) - 1$.

Implicit-explicit integrators

- By induction, we define the terms Z_ℓ in the formal series
- All the Z_ℓ are symmetric operators.
- Analytic estimates :

$$\|Z_\ell\|_\alpha \leq \left(C\|V\|_\alpha\right)^\ell$$

- The series $Z(t) = \sum_{t\geq 0} t^\ell Z_\ell$ converges for

$$t \leq \tau_0 \sim \|V\|_\alpha^{-1}.$$

- $R(-it\Delta)\exp(itV) = \exp(iZ(t))$. No remainder term.

Modified energy

Theorem (Debussche & Faou 2008)

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 potential
- $\langle u|S(\tau)|u\rangle$ invariant of the numerical scheme
- No residual term.
- Backward error analysis result.
- Same result for standard 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 :

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

Theorem

$\beta \in [0, 1]$.

$$\Big| \langle u | S(\tau) | u \rangle - \langle u | -\Delta + V | u \rangle \Big| \leq C\tau^\beta \|u\|^2_{H^{1+\beta}} .$$

- Proof : $|\arctan(x) - x| \leq x^3/3$...

Long time bounds

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

Control of the H^1 norm for low modes and L^2 norm for high modes .

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 $u(t,x) \in \mathbb{C}$, $x \in \mathbb{T}^d$.

- Hamiltonian

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

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

$$\begin{aligned} H(u,\bar{u}) &= T(u,\bar{u}) + P(u,\bar{u}) \\ &= \sum_{k \in \mathbb{Z}^d} |k|^2 |u_k|^2 + \frac{1}{2} \sum_{k_1 + k_2 - \ell_1 - \ell_2 = 0} u_{k_1} u_{k_1} \bar{u}_{\ell_1} \bar{u}_{\ell_2}. \end{aligned}$$

Cubic nonlinear Schrödinger equation

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

$$\dot{u}_k = -i \frac{\partial H}{\partial \bar{u}_k}(u, \bar{u}),$$

$$\dot{u}_k = -i|k|^2 u_k - i \sum_{k=k_1-\ell_1+k_2} u_{k_1} \bar{u}_{\ell_1} u_{k_2}.$$

Splitting methods

- Hamiltonian $H = T + P$. Splitting methods :

$$\Phi^\tau = \phi_P^\tau \circ \phi_{A_0}^1$$

- Filtered operator $A_0 = \beta(\tau\Delta)$ with eigenvalues

$$\lambda_k = \beta(\tau|k|^2), \quad k \in \mathbb{Z}^d$$

- Convergent scheme for smooth solutions : $\beta(x) \simeq x + o(x)$

Method	$\beta(x)$
Splitting + CFL	$\beta(x) = x\mathbb{1}_{x<c}(x)$
Mid-split	$\beta(x) = 2\arctan(x/2)$
Mid-split + CFL	$\beta(x) = 2\arctan(x/2)\mathbb{1}_{x<c}(x)$
New scheme	$\beta(x) = \tau^\beta \arctan(\tau^{-\beta}x), \quad \beta \in (0,1)$

Modified energy

As in the linear case, we look for a (polynomial) Hamiltonian $Z(t)$ such that

$$\forall\, t \in (0,\tau) \quad \phi_P^t \circ \phi_{A_0}^1 = \phi_{Z(t)}^1$$

Equation :

$$Z'(t) = \sum_{n\geq 0} \frac{B_n}{n!} \mathrm{ad}^n_{iZ(t)}(P).$$

where this time

$$\mathrm{ad}_K(G) = \{K, G\} = i \sum_{k\in\mathbb{Z}^d} \frac{\partial K}{\partial u_k}\frac{\partial G}{\partial \bar{u}_k} - \frac{\partial K}{\partial \bar{u}_k}\frac{\partial G}{\partial u_k}$$

Formal series : $Z(t) = A_0 + tZ_1 + t^2 Z_2 + \cdots$

Modified energy

Cubic NLS :

$$P = \sum_{k_1+k_2-\ell_1-\ell_2=0} u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2}$$

First term in the expansion :

$$Z_1 = \sum_{k_1+k_2-\ell_1-\ell_2=0} \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{A_0}^k (u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2})$$

Action of $A_0 = \sum_k \lambda_k |u_k|^2$:

$$\{A_0, u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2}\} = i\Omega(k_1, k_2, \ell_1, \ell_2) u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2}$$

where

$$\Omega(k_1, k_2, \ell_1, \ell_2) = \lambda_{k_1} + \lambda_{k_2} - \lambda_{\ell_1} - \lambda_{\ell_2}$$

Modified energy

Convergence : $\Omega(k_1, k_2, \ell_1, \ell_2) < 2\pi$.

$$Z_1 = \sum_{k_1+k_2-\ell_1-\ell_2=0} \left(\sum_{k=0}^{\infty} \frac{B_k}{k!} \Omega(k_1, k_2, \ell_1, \ell_2)^k \right) u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2}$$

- Splitting : with CFL

$$|\Omega(k_1, k_2, \ell_1, \ell_2)| = |\tau |k_1|^2 + \tau |k_2|^2 - \tau |\ell_1|^2 - \tau |\ell_2|^2| \leq 2c < 2\pi$$

- Midpoint : always satisfied

$$|\Omega(k_1, k_2, \ell_1, \ell_2)| = |2\arctan(\tau |k_1|^2/2) + 2\arctan(\tau |k_2|^2/2) - 2\arctan(\tau |\ell_1|^2/2) - 2\arctan(\tau |\ell_2|^2/2))| < 2\pi$$

- New scheme : no problem $\lambda_k = \sqrt{\tau} \arctan(\sqrt{\tau} |k|^2) \leq \pi \sqrt{\tau}/2$

$$\Longrightarrow |\Omega(k_1, k_2, \ell_1, \ell_2)| \leq 2\pi\sqrt{\tau} < 2\pi$$

Modified energy

First term (cubic NLS) :

$$Z_1 = \sum_{k_1+k_2-\ell_1-\ell_2=0} \left(\frac{i\Omega(k_1,k_2,\ell_1,\ell_2)}{e^{i\Omega(k_1,k_2,\ell_1,\ell_2)}-1} \right) u_{k_1} u_{k_2} \bar{u}_{\ell_1} \bar{u}_{\ell_2}$$

- Z_1 : Control of the small denominator at the order 4.
- Z_2 : defined similarly, but of degree 6.
- By induction : Z_n sum of monomials $u_{k_1} \cdots u_{k_p} \bar{u}_{\ell_1} \cdots \bar{u}_{\ell_p}$, with $2p = 2n+2$

$$\Omega(\mathbf{k}, \boldsymbol{\ell}) = \lambda_{k_1} + \cdots + \lambda_{k_p} - \lambda_{\ell_1} - \cdots - \lambda_{\ell_p}$$

Solution of the recursive equations : as long as

$$|\Omega(\mathbf{k}, \boldsymbol{\ell})| < 2\pi$$

Solution of the recursive equations

Theorem

Assume

$$|\Omega(\mathbf{k},\ell)| < 2\pi.$$

for multiindex of size $2p \leq r$. Then for $n \leq N := r/2 - 1$ we can define polynomials Z_n of degrees $2n+2$ solving the formal problem, and such that for $n \leq N$,

$$\|Z_n\| \leq (Cn)^n$$

- Norm on polynomials : sup of the coefficients.
- Key lemma :

$$\|\{P,Q\}\| \leq 2nm\|P\|\,\|Q\|$$

if P is of degree n, and Q of degree m.

Polynomial Hamiltonian

- Function space : Wiener algebra ℓ^1.

$$\|u\|_{\ell^1} := \sum_{k\in\mathbb{Z}^d} |u_k|.$$

- For a homogeneous polynomial of degree n, $\|P\|$ = sup of the coefficients

$$|P(u)| \leq \|P\| \, \|u\|_{\ell^1}^n , \quad \text{and} \quad \|X_P(u)\|_{\ell^1} \leq 2n\|P\| \, \|u\|_{\ell^1}^n .$$

- The Hamiltonian $Z^N := A_0 + tZ_1 + \cdots t^N Z_N$ acts on ℓ^1. We can derive estimates on the flow of the modified energy.
- Possible extension to ℓ_s^1 : $\|u\|_{\ell_s^1} := \sum_{k\in\mathbb{Z}^d} |k|^s |u_k|$.

Modified flow

Theorem (Faou & Grébert 2009)

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

$$\|\phi_P^\tau \circ \phi_{A_0}^1(u) - \phi_{H_\tau}^\tau(u)\|_{\ell^1} \le \tau^{N+1}(CN)^N.$$

$$H_\tau(u,\bar{u}) = \sum_{k\in\mathbb{Z}^d} \frac{1}{\tau}\beta(\tau|k|^2)|u_k|^2 + \sum_{k_1+k_2-\ell_1-\ell_2=0} \frac{i\Omega(k_1,k_2,\ell_1,\ell_2)}{e^{i\Omega(k_1,k_2,\ell_1,\ell_2)}-1} u_{k_1}u_{k_2}\bar{u}_{\ell_1}\bar{u}_{\ell_2} + \mathcal{O}(\tau)$$

N given by the non resonance condition $|\Omega(\mathbf{k},\ell)| < 2\pi$.
$\mathrm{length}(\mathbf{k},\ell) \le r = 2N+2$.

Exponential estimates

- N depends in general on a CFL condition.
- In the case

$$\beta(x) = \sqrt{\tau}\arctan(x/\sqrt{\tau})$$

we have

$$\lambda_k = \sqrt{\tau}\arctan(\sqrt{\tau}|k|^2). \quad \Longrightarrow |\Omega(\mathbf{k},\ell)| \leq r\sqrt{\tau}\frac{\pi}{2} \leq \pi$$

for $r \simeq 1/\sqrt{\tau} \simeq N$.

Theorem

There exists τ_0, such that for all $\tau \leq \tau_0$, and all $u \in B_M$, we have

$$\|\phi_P^\tau \circ \phi_{A_0}^1(u) - \phi_{H_\tau}^\tau(u)\|_{\ell^1} \leq \tau \exp(-(\tau_0/\tau)^{1/2}).$$

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

Preservation of the modified energy

Corollary

Let $u^0 \in \ell^1$ and the sequence u^n defined by

$$u^{n+1} = \phi_P^\tau \circ \phi_{A_0}^1(u^n), \quad n \geq 0.$$

Assume that for all n, $u^n \in B_M \subset \ell^1 \subset L^\infty$. Then

$$H_\tau(u^n) = H_\tau(u^0) + \mathcal{O}(\tau)$$

for $n\tau \leq C_N \tau^{-N}$.

{EC

Long time bounds

In particular for the implicit-explicit integrator :

$$\sum_{k\in\mathbb{Z}^d} \frac{1}{\tau}\arctan(\tau|k|^2)|u_k^n|^2.$$

is bounded over long time.

Corollary

Assume $u^0 \in H^1$ and that u^n remains bounded in ℓ^1. Then

$$\sum_{|k|<\tau^{-1/2}} |k|^2|u_k^n|^2 + \frac{1}{\tau}\sum_{|k|\geq\tau^{-1/2}} |u_k^n|^2 \leq C$$

over long time $n\tau \leq C_N\tau^{-N}$.

Fully discrete solution

- Pseudo spectral collocation method : aliasing problem.
- If $u^{K,n}$ is the polynomial fully discrete solution : Bounds for

$$\sum_{|k|<K=c\tau^{-1/2}} |k|^2|u_k^{K,n}|^2 = \|u^{K,n}\|_{H^1}^2$$

- In dimension 1 : $\|u\|_{\ell^1} \leq \|u\|_{H^1}$.
  Global existence of H^1 small solutions of NLS. Discrete analog :

Theorem (dimension 1)

There exists ϵ_0 such that if $\epsilon < \epsilon_0$ and $\|u^{K,0}\|_{H^1} \leq \epsilon$, then

$$\forall\, n\tau \leq C_N\tau^{-N} \qquad \|u^{K,n}\|_{H^1} \leq C\epsilon$$

where C does not depend on K.

Extensions

Extensions

- Polynomial nonlinearity of degree r_0.
- Nonlinear wave equations.

Open questions :

- Other space discretization (FEM, sparse grids ?)
- Validity for any symplectic RK method ?
- Orbital stability of the numerical solitary wave ?
  (in progress with Bambusi & Grébert)
- Periodic solutions for the modified Hamiltonian ? KAM ?

Web Link :

`http ://www.irisa.fr/ipso/perso/faou/ETH/ETH.html`