Resonances in long time integration of the nonlinear Schrödinger equation

Erwan Faou

INRIA & ENS Cachan Bretagne

Oberwolfach, 22 March 2011

Cubic nonlinear Schrödinger equation

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

Wave function $u(t,x) \in \mathbb{C}$, $x \in \mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$.

- Preservation of the L^2 norm : $\|u(t)\|_{L^2}^2 = \|u(0)\|_{L^2}^2$.
- Hamiltonian preserved for all times

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

- $\lambda > 0$: focusing, $\lambda < 0$: defocusing.

Cubic nonlinear Schrödinger equation

Decomposition $u(t,x) = \sum_{j\in\mathbb{Z}} \xi_j(t) e^{ijx}$,

$$
\begin{aligned}
H(\xi,\bar\xi) &= T(\xi,\bar\xi) + P(\xi,\bar\xi) \\
&= \sum_{j\in\mathbb{Z}} |j|^2 |\xi_j|^2 + \frac{\lambda}{2} \sum_{\substack{j,k,\ell,m\in\mathbb{Z} \\ j=k-\ell+m}} \xi_k \xi_m \bar\xi_\ell \bar\xi_j .
\end{aligned}
$$

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

$$
\dot\xi_j = -i|j|^2 \xi_j - i\lambda \sum_{j=k-\ell+m} \xi_k \bar\xi_\ell \xi_m = -i \frac{\partial H}{\partial \bar\xi_j}(\xi,\bar\xi)
$$

Semi-discrete system

Space approximation : Fourier pseudo-spectral collocation method :

$$U^K(t,x) = \sum_{j \in B^K} \xi_j^K(t) e^{ij\cdot x}$$

satisfying NLS at the grid points $x_j = 2j\pi/K \in [-\pi,\pi]$, $j \in B^K$

- $K = 2P+1$ odd : $B^K = \{-P, \cdots, P\}$
- $K = 2P$ even : $B^K = \{-P, \cdots, P-1\}$.

Semi-discrete system

Space discretized Hamiltonian :

$$\begin{aligned} H^K(\xi,\bar\xi) &= T^K(\xi,\bar\xi) + P^K(\xi,\bar\xi) \\ &= \sum_{k\in B^K} |k|^2 \|\xi_k|^2 + \frac{\lambda}{2} \sum_{\substack{k,m,\ell,j\in B^K \\ k+m-\ell-j\in K\mathbb{Z}}} \xi_k \xi_m \bar\xi_\ell \bar\xi_j . \end{aligned}$$

Aliasing problem

Semi-discrete NLS : For all $j \in B^K$

$$\dot\xi_j^K = -i|j|^2 \xi_j^K - i\lambda \sum_{\substack{j=k-\ell+m+\delta K \\ \delta\in\{0,\pm1\}}} \xi_k^K \bar\xi_\ell^K \xi_m^K .$$

Splitting schemes

Stepsize τ.Splitting schemes

$$\xi^{K,n+1} = \varphi^{\tau}_{P^K} \circ \varphi^{\tau}_{T^K}(\xi^{K,n}).$$

Practical implementation : Using FFT

- $\varphi^{\tau}_{P^K}$ diagonal on the grid $x_j \in [-\pi, \pi]$

$$i\partial_t u = |u|^2 u \Longrightarrow u(t,x) = e^{-it|u^0(x)|^2} u^0(x)$$

- $\varphi^{\tau}_{T^K}$ diagonal in Fourier

$$i\partial_t \xi_j = |j|^2 \xi_j \Longrightarrow \xi_j(t) = e^{-it|j|^2} \xi_j(0)$$

Possible use of implicit scheme for the linear part (midpoint)

Backward error analysis for PDEs

Theorem (Faou & Grébert 2009)

M fixed. There exists C such that for all N, K, τ satisfying

$$\mathrm{CFL} := \tau \frac{K^2}{2} < \frac{2\pi}{N+1},$$

there exists a polynomial Hamiltonian H_τ^K such that for all $\xi \in B_M = \{\, \xi \in \ell^1 \mid \|\xi\|_{\ell^1} \leq M \,\}$, we have

$$\|\phi_{P^K}^\tau \circ \phi_{T^K}^\tau(\xi) - \phi_{H_\tau^K}^\tau(\xi)\|_{\ell^1} \leq \tau^{N+1}(CN)^N.$$

$\|\xi\|_{\ell^1} := \sum_{k\in\mathbb{Z}} |\xi_k|$ *Wiener algebra.*

Backward error analysis for PDEs

Modified Hamiltonian

$$H_\tau^K(\xi,\bar\xi) = \sum_{k\in B^K} |k|^2|\xi_k|^2 + \frac{1}{2}\sum_{\substack{k,m,\ell,j\in B^K\\ k+m-\ell-j\in K\mathbb{Z}}} \frac{i\tau\Omega_{km\ell j}}{e^{i\tau\Omega_{km\ell j}}-1}\xi_k\xi_m\bar\xi_\ell\bar\xi_j + \mathcal{O}(\tau)$$

with $\Omega_{km\ell j} = |k|^2+|m|^2-|\ell|^2-|m|^2$.

- Also valid for implicit-explicit schemes (better CFL condition) but numerical eigenvalues (instead of $|k|^2$)

$$\lambda_k = \frac{2}{\tau}\arctan\left(\frac{\tau|k|^2}{2}\right)$$

- Valid for semilinear Hamiltonian PDEs with discrete spectrum.
- Linear case : Debussche & Faou 06

CFL conditions

τ^{N+1}	Standard	Implicit-explicit
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 solution

- If $u^{K,n} = \sum_{k\in B^K} \xi_k^{K,n} e^{ikx}$ is the polynomial fully discrete solution : Preservation of the modified energy as long as the solution remains bounded in ℓ^1.
- 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.

Cubic NLS on the torus : small solutions

Cubic NLS on $\mathbb{T}^d$: Behavior of solutions over long time ?
Small initial data after scaling : $\varepsilon << 1$.

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u, \quad u(0,x) = u_0(x) \simeq 1.$$

In Fourier

$$u(t,x) = \sum_{j \in \mathbb{Z}^d} e^{ij\cdot x} u_j(t)$$

$$i\dot{u}_j = |j|^2 u_j + \varepsilon \sum_{j=k+\ell-m} u_k u_\ell \bar{u}_m = \frac{\partial H}{\partial \bar{u}_j}(u)$$

$|j|^2 = j_1^2 + \cdots + j_d^2$. Hamiltonian

$$H(u,\bar{u}) = \sum_{j\in\mathbb{Z}^d} |j|^2 |u_j|^2 + \frac{\varepsilon}{2} \sum_{j+k=\ell+m} u_j u_k \bar{u}_\ell \bar{u}_m$$

Cubic NLS on the torus

$$i\partial_t u = -\Delta u + Vu + \varepsilon |u|^2 u.$$

With potential : Stability results.

- Bourgain, Kuksin, Craig & Wayne, Pöschel, etc...
- KAM (Eliasson & Kuksin 10)
- Birkhoff normal forms (Bambusi & Grébert 06)
- Nekhoroshev-like estimates (Faou & Grébert 10)

Typical result : $\|u(0)\|_{H^s} = 1$ then $\|u(t)\|_{H^s} \leq 2$ and

$$\left| |u_j(t)|^2 - |u_j(0)|^2 \right| \leq \frac{\varepsilon}{|j|^{2s}}, \quad t \leq \varepsilon^{-r}$$

Optimization of the constants : $t \leq \varepsilon^{-|\ln \varepsilon|^\beta}$.

Cubic NLS on the torus

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u.$$

Without potential. Dimension 1 :

- Integrable system (Zakharov & Shabat 84).
- Global Birkhoff (action-angle) variables (Kappeler, Pöschel, Grébert 10).
- Solitary waves stability (Gallay & Haragus 08).
- More general nonlinearities : KAM (Kuksin, Pöschel 96).

$\Longrightarrow$ Preservation of the actions over long time

Cubic NLS on the torus

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u.$$

Without potential. Dimension $d \geq 2$:

- There exist many quasiperiodic solutions (Wang, Procesi & Procesi, Geng & Xou & You 2010).
- For all M, there exists u_0 and T such that $\|u_0\|_{H^s} \leq 1$ and $\|u(T)\|_{H^s} \geq M$.
(Colliander, Keel, Staffilani, Takaoka, Tao 10)

Cubic NLS on the torus

$$i\partial_t u = -\Delta u + Vu + \varepsilon|u|^2 u, \quad u(0,x) = u_0(x) \simeq 1.$$

Numerical analysis ?

With potential :

- Faou, Grébert & Paturel using normal forms
- Gauckler & Lubich using Modulated Fourier Expansion.

Without potential

- Backward error analysis (with Grébert). Almost global existence in H^1 in dimension 1.
- Stability of numerical solitons (with Bambusi & Grébert). Dimension 1.

An approximation result

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u.$$

Theorem

The solution $u(t,x)$ in Fourier satisfies

$$u_j(t) = e^{-it|j|^2} v_j(\varepsilon t) + \mathcal{O}(\varepsilon)$$

for $t \leq T/\varepsilon$, where $v_j(\tau)$ solves

$$i \frac{\mathrm{d}}{\mathrm{d}\tau} v_j(\tau) = \sum_{\substack{j=k+\ell-m \\ |j|^2=|k|^2+|\ell|^2-|m|^2}} v_k(\tau) v_\ell(\tau) \bar{v}_m(\tau)$$

Proof : Normal forms, WKB, Averaging, WNLGO, MFE, etc...

An approximation result

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u$$

We seek $u_j(t)$ under the form $u_j(t) = e^{-it|j|^2} v_j(\varepsilon t)$.
Setting $\tau = \varepsilon t$,

$$i \frac{\mathrm{d}}{\mathrm{d}\tau} v_j(\tau) = \sum_{j=k+\ell-m} v_k(\tau) v_\ell(\tau) \bar{v}_m(\tau) e^{-i\frac{\tau}{\varepsilon}(|k|^2+|\ell|^2-|m|^2-|j|^2)}$$

Equivalently

$$iv_j(\tau) = iv_j(0) + \sum_{j=k+\ell-m} \int_0^\tau v_k(s) v_\ell(s) \bar{v}_m(s) e^{-i\frac{s}{\varepsilon}(|k|^2+|\ell|^2-|m|^2-|j|^2)} \mathrm{d}s.$$

An approximation result

Here we use

$$\int_0^t U(s)e^{i\frac{s}{\varepsilon}\Omega}\mathrm{d}s = \begin{cases} \int_0^t U(s)\mathrm{d}s & \text{if} \quad \Omega = 0 \\ \mathcal{O}(\varepsilon) & \text{if} \quad \Omega \neq 0. \end{cases}$$

We obtain

$$iv_j(\tau) = iv_j(0) + \sum_{\substack{j=k+\ell-m \\ |j|^2=|k|^2+|\ell|^2-|m|^2}} \int_0^\tau v_k(s)v_\ell(s)\bar{v}_m(s)\mathrm{d}s + \mathcal{O}(\varepsilon).$$

Resonant case : no small divisors issues.

Resonant system

Resonant system :

$$i\dot{v}_j = \sum_{\substack{j=k+\ell-m \\ |j|^2=|k|^2+|\ell|^2-|m|^2}} v_k v_\ell \bar{v}_m$$

Hamiltonian system with Hamiltonian

$$Z(v) = \frac{1}{2} \sum_{\substack{k+\ell-j-m=0 \\ |k|^2+|\ell|^2-|j|^2-|m|^2=0}} v_k v_\ell \bar{v}_j \bar{v}_m$$

Resonance modulus

$$\mathcal{K} = \{|j|^2 + |k|^2 - |\ell|^2 - |m|^2 = 0 \quad \text{and} \quad j + k - \ell - m = 0\}.$$

Lemma

A quadruplet $(j, k, \ell, m) \in \mathbb{Z}^d$ is in $\mathcal{K}$ when

- *The endpoints of the vectors j, k, ℓ, m form four corners of a non-degenerate rectangle with j and k opposing each other*
- *The situation corresponds to one of the two degenerate cases : $(j = \ell, k = m)$, or $(j = m, k = \ell)$.*

Resonance modulus

Proof : $|j+k|^2 = |\ell+m|^2$ implies $j \cdot k = \ell \cdot m$. Then

$$\begin{aligned}(j-m)\cdot(k-m) &= j\cdot k - m\cdot(j+k-m)\\ &= -m\cdot(j+k-\ell-m) = 0.\end{aligned}$$

In dimension 1 : no rectangles. The resonant Hamiltonian

$$Z = \frac{\lambda}{2}\Big(\sum_j |u_j|^4 + 2\sum_{j\neq k}|u_j|^2|u_k|^2\Big)$$

only depends on the **actions** $I_j(u) = |u_j|^2$. In particular

$$\{I_j, Z\} = 0.$$

Hence $|v_j(\tau)|^2 = |u_j(\varepsilon t)|^2 = cst$ for $t \le T/\varepsilon$.

Resonance modulus

Theorem (dimension 1)

There exists ε_0 *and a constant* c *such that if* $\|u_0\|_{H^1} \leq 1$, *then for* $\varepsilon \leq \varepsilon_0$, *if* $t \leq c\varepsilon^{-1}$,

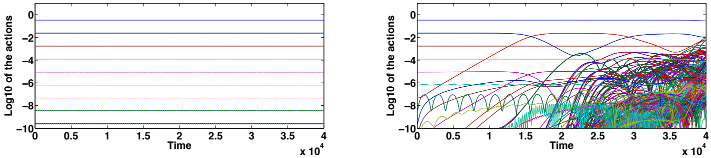
$$\left| |u_j(t)|^2 - |u_j(0)|^2 \right| \leq \varepsilon.$$

Natural question : can we reproduce this phenomenon numerically ?

Numerical preservation of the actions

Resonances because of the stepsize : $u^0(x) = 1/(2 - \cos(x))$, $\varepsilon = 0.01$, $K = 512$ grid points.

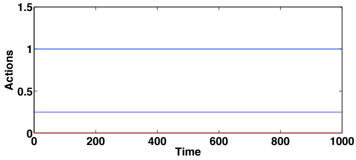
$$\tau = 0.09 \quad \text{and} \quad \tau = \frac{1}{12^2 - 5^2 - 7^2} \simeq 0.0898\ldots$$

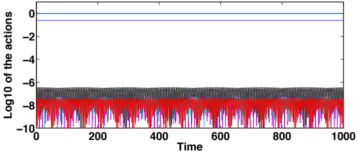


Plot : $\log|\xi_j^{K,n}|^2$.

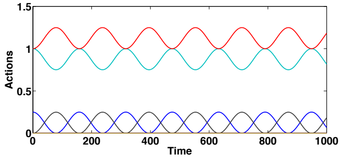
Numerical preservation of the actions

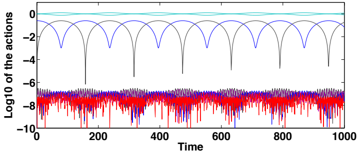
Aliasing instabilities :
$\varepsilon = 0.01$, $\tau = 10^{-3}$, $u^0(x) = 2\sin(10x) - 0.5e^{i7x}$.
$K = 31$:





$K = 34 = 2 \times 17$. Preservation of the super actions $|\xi_j|^2 + |\xi_{-j}|^2$



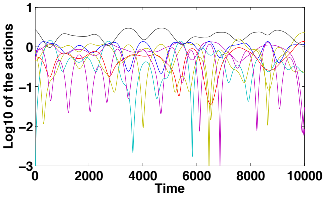


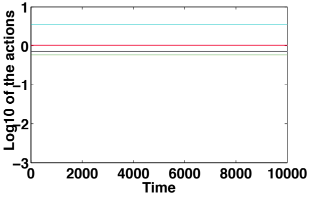
Numerical preservation of the actions

Aliasing instabilities :
$\tau = 0.001$, $\varepsilon = 0.05^2$,

$$u^0(x) = 0.9\cos(-5x) + \sin(14x) + 1.1\exp(-10ix) + 1.2\cos(-11x).$$

$K = 30 = 2 \times 3 \times 5$ and $K = 31$.





Numerical Resonance modulus

Modified energy

$$H_\tau^K = \sum_{j\in B^K} j^2|u_j|^2 + \frac{\varepsilon}{2} \sum_{\substack{j+k=\ell+m+\delta K\\ \delta=0,\pm1}} \frac{i\tau\Omega_{jk\ell m}}{e^{i\tau\Omega_{jk\ell m}}-1} u_j u_k \bar{u}_\ell \bar{u}_m + \mathcal{O}(\varepsilon^2 u^6).$$

Approximation result $\Longrightarrow$ Numerical resonance modulus

$$\mathcal{K}^K = \{j,k,\ell,m \in (B^K)^4 \mid j^2+k^2-\ell^2-m^2=0 \\ \text{and} \quad j+k-\ell-m=\delta K, \quad \delta\in\{0,\pm1\}\}.$$

Numerical Resonance modulus

Lemma

The following holds :

(i) *Assume that* $K \geq 3$ *is a* **prime** *number. Then* $\mathcal{K}^K$ *contains only terms such that* $j = \ell$ *and* $k = m$*, or* $j = m$ *and* $k = \ell$*.*

(ii) *Assume that* $K/2 \geq 3$ *is a* **prime** *number. Then* $\mathcal{K}^K$ *contains only terms such that* $j = \ell$ *and* $k = m$*, or* $j = m$ *and* $k = \ell$*, and the terms such that* $j = -m$ *and* $k = -\ell$*, or* $j = -\ell$ *and* $k = -m$*, under the constraint* $j + k = \delta K/2$*,* $\delta = \pm 1$*.*

In the other cases : strongly nonlinear interactions always possible.

Fully discrete preservation of the actions

Theorem

Assume that K is a **prime number**, *and let $u^{K,n} = \sum_{k\in\mathbb{Z}} \xi_j^{K,n} e^{ijx}$ the fully discrete solution after n iterations of a splitting algorithm. Then for ε and τ sufficiently small, if $\|u_0\|_{H^1} \leq 1$, then for $n\tau \leq c\varepsilon^{-1}$,*

$$\forall j \in B^K, \quad \left| |\xi_j^{K,n}(t)|^2 - |\xi_j^{K,0}(0)|^2 \right| \leq \varepsilon.$$

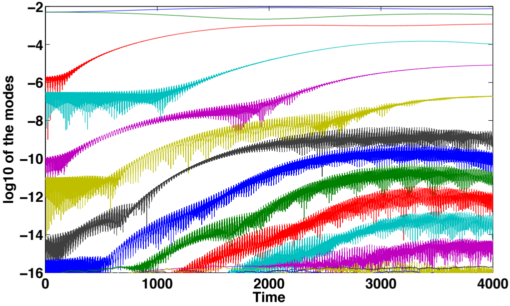
where

Same result if $K = 2P$, P prime, and for the super actions.

Dimension two

$$i\partial_t u = -\Delta u + \varepsilon |u|^2 u$$

Generic initial data : preservation of the regularity over very long time.
But : initial data $1 + 2\cos(x) + 2\cos(y)$ we have



Dimension two

To prove this : let us go back to the resonant system

$$u(t) \simeq \sum_j v_j(\varepsilon t) e^{-i|j|^2 t} + \mathcal{O}(\varepsilon), \quad t \leq T/\varepsilon.$$

$$i\dot{v}_j = \sum_{\substack{|j|^2=|k|^2+|\ell|^2-|m|^2 \\ j=k+\ell-m}} v_k v_\ell \bar{v}_m.$$

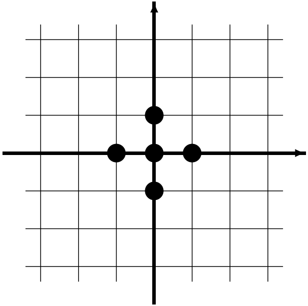
Idea : Taylor expansion of

$$v_j(\varepsilon t) = v_j(0) + \sum_{n\geq 1} \varepsilon^n t^n \frac{\mathrm{d}^n}{\mathrm{d}t^n} v_j(0)$$

.

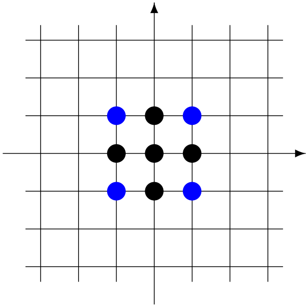
Simulating energy cascades

$v_j(0)$



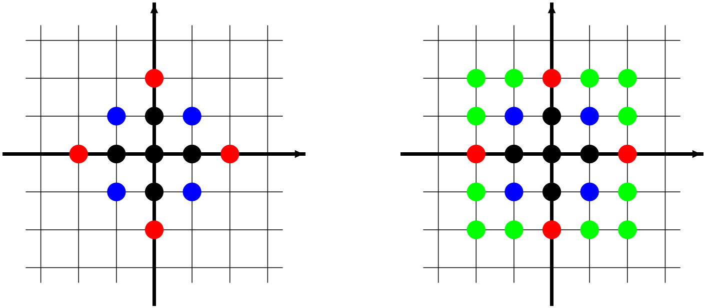
Simulating energy cascades

$\frac{\mathrm{d}}{\mathrm{d}t} v_j(0)$, by the rectangle rule



Simulating energy cascades

Next two steps :



Energy cascades

Dynamics of the modes : In general very complicated
But not for the *extremal modes* :

$$\mathcal{N}_* = \{(0, \pm 2^p), (\pm 2^p, 0), (\pm 2^p, \pm 2^p), (\mp 2^p, \pm 2^p), \;\; p \in \mathbb{N}\}$$

Energy cascade

$$i\partial_t u = -\Delta u + \varepsilon\lambda |u|^2 u.$$

Theorem (Carles & Faou 2010)

Let $u^0(x,y) = 1 + 2\cos x + 2\cos y$. *Then*

$$\forall \gamma \in]0,1[,\ \forall \theta < \frac{1}{4},\ \forall \alpha > 0, \quad \exists \varepsilon_0, \quad \forall \varepsilon \in]0,\varepsilon_0],$$

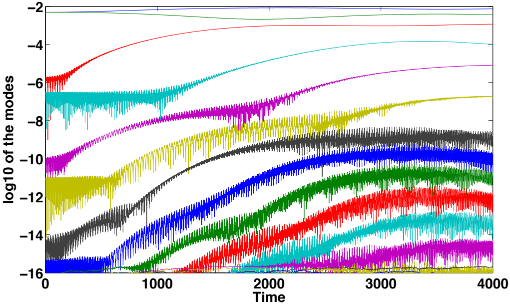
$$\forall j \in \mathcal{N}_*,\ |j| < \alpha \left(\log \frac{1}{\varepsilon}\right)^{\theta}, \quad \left| u_j \left(\frac{2}{\varepsilon^{1-\gamma/(|j|^2-1)}} \right) \right| \geqslant \frac{\varepsilon^{\gamma}}{4}.$$

Sequence of increasing times $t_j^\varepsilon = \frac{2}{\varepsilon^{1-\gamma/(|j|^2-1)}} \to \frac{2}{\varepsilon}$, $|j| \to \infty$.

Compare with the case with potential (or dimension 1) :

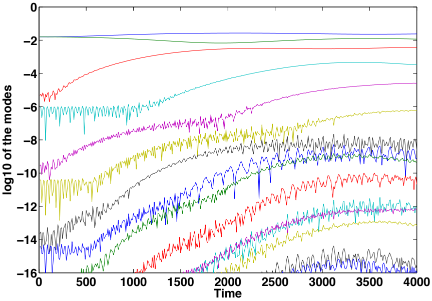
$$|u_j(t)| \leq \varepsilon, \quad t \leq \varepsilon^{-r}.$$

Energy cascade



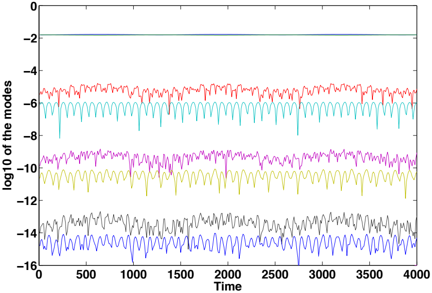
$$u(0) = (1 + e^{ix} + e^{-ix} + e^{iy} + e^{-iy})$$

Simulating energy cascades



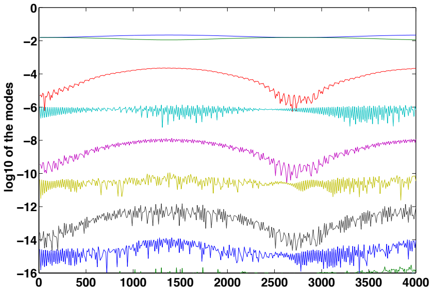
Computation with an explicit splitting algorithm
$\lambda_k = \tau |k|^2$, $\tau = 0.1$, grid 128×128.

Simulating energy cascades



Computation with an implicit-explicit splitting algorithm
$\tau = 0.1$, grid 128×128.

Simulating energy cascades



Computation with an implicit-explicit splitting algorithm
$\tau = 0.05$, grid 128×128.

Simulating energy cascades

Explanation : for implicit-explicit schemes, Backward error analysis :

$$H_\tau = \sum_{j \in B^K} \lambda_k |u_j|^2 + \frac{\varepsilon}{2} \sum_{\substack{j+k=\ell+m+\delta K \\ \delta=0,\pm 1}} \frac{i\Lambda_{jk\ell m}}{e^{i\Lambda_{jk\ell m}} - 1} u_j u_k \bar{u}_\ell \bar{u}_m + \mathcal{O}(\varepsilon^2 u^6).$$

$\Lambda_{jk\ell m} = \lambda_j + \lambda_k - \lambda_\ell - \lambda_m$ with

$$\lambda_k = 2 \arctan(\tau |k|^2).$$

Implicit midpoint propagator in Fourier

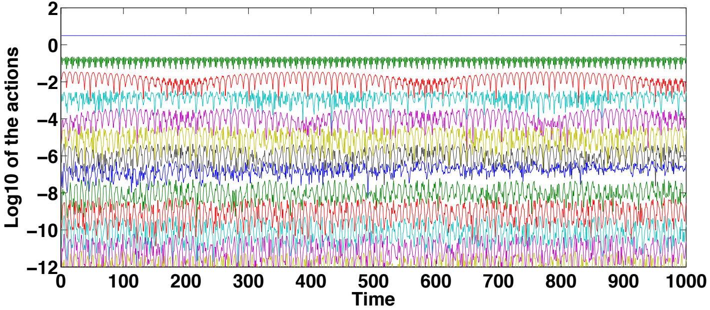
$$\frac{1 + i\tau|k|^2/2}{1 - i\tau|k|^2/2} = \exp(2i \arctan(\tau|k|^2)).$$

Implicit schemes cannot reproduce the correct energy exchanges...

Plane wave stability

$$i\partial_t u = -\Delta u + \lambda |u|^2 u$$

Initial data localized around the $(0,0)$ mode
$u^0(x,y) = \pi + \varepsilon(2\cos(x) + 2\cos(y))$



Plane wave stability

$$\partial_t u = -\Delta u + \lambda |u|^2 u, \quad \langle u \rangle = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} u(x) \mathrm{d}x$$

Theorem (Faou, Gauckler & Lubich 2011)

Let r be fixed. For **generic** *ρ such that*

$$1 + 2\lambda\rho^2 > 0,$$

for $s \geq s_0$, if

$$\|u(0)\|_{L^2} = \rho \quad \text{and} \quad \|u^0 - \langle u^0 \rangle\|_{H^s} = \varepsilon \leq \varepsilon_0,$$

then

$$\|u(t) - \langle u(t) \rangle\|_{H^s} \leq 2\varepsilon \quad \text{for} \quad t \leq C\varepsilon^{-r}.$$

Conclusions

- Numerical simulation of resonant system can lead to strong instabilities (times step, number of grid points).
- The linear frequencies have to be carefully approximated (no implicit solvers, low CFL).
- Main tool : backward error analysis for PDE under CFL.
- Many open problems for the continuous case and the numerical approximations.
  Numerical simulations are helpful for numerical analysis and for the search of new nonlinear phenomena.