Numerical methods for the stochastic Schödinger equation

Laurent Di Menza

Laboratoire de Mathématiques - Université de Reims

Joint work with A. Debussche and M. Barton-Smith

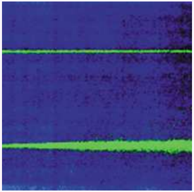
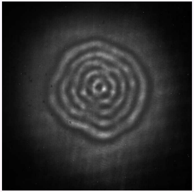
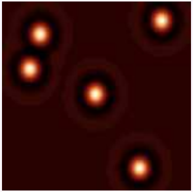
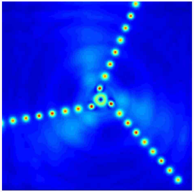
Workshop *The Stochastic Schrödinger equation in selected physics models*

CEA/SphN, F-91191 Gif-sur-Yvette, December 6-7th, 2011

Outline of the talk

1. Physical context and mathematical model

Physical context : electromagnetical wave propagation in nonlinear media, with various applications (optics, telecommunications).

Time evolution of physical quantities (density, electric field) are governed by complex mathematical models (coupling between Maxwell system and law of state in the nonlinear media).

- Assumptions are needed in order to obtain a reasonable model.
- Even in this case, we use numerical tools to perform simulations.

A mathematical model

Nonlinear Schrödinger equation : *ideal* mathematical model involved in many physical contexts : nonlinear optics, plasmas physics, fluids, quantum physics, etc.

(NLS) $$i\frac{\partial \psi}{\partial t} + \Delta\psi + |\psi|^{2\sigma}\psi = 0$$

with $\psi = \psi(t,x) \in \mathbb{C}$, $x \in \mathbb{R}^d$ and $\sigma > 0$.

Cauchy problem in $H^1(\mathbb{R}^d)$: (Ginibre-Velo, Strauss, etc.)

- If $\sigma < 2/(d-2)$, locally well-posed : if $\psi_0 \in H^1(\mathbb{R}^d)$, $\exists\, T > 0$ and $\exists !\, \psi \in \mathcal{C}(0,T;H^1(\mathbb{R}^d))$ solves (NLS) with $\psi(0) = \psi_0$.
- If $\sigma < 2/d$, globally well-posed : if $\psi_0 \in H^1(\mathbb{R}^d)$, $\exists !\, \psi \in \mathcal{C}(\mathbb{R}^+;H^1(\mathbb{R}^d))$ solves (NLS) with $\psi(0) = \psi_0$.

Solutions properties

Conserved quantities :

- $M(\psi) = \int_{\mathbb{R}^d} |\psi(x)|^2 \, dx$ (mass),
- $H(\psi) = \int_{\mathbb{R}^d} \|\nabla \psi(x)\|^2 \, dx - \dfrac{1}{\sigma + 1} \int_{\mathbb{R}^d} |\psi(x)|^{2(\sigma+1)} \, dx$ (energy).

Specific solutions :

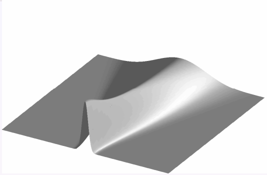
- Stationary states $\psi(t,x) = e^{i\omega t} u(x)$ (global in $H^1(\mathbb{R}^d)$), where u solves the elliptic problem

$$-\omega u + \Delta u + |u|^{2\sigma} u = 0, \quad x \in \mathbb{R}^d.$$

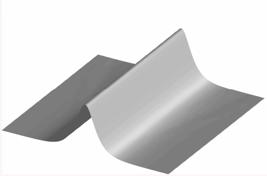
- Explosive solutions in $H^1(\mathbb{R}^d)$ if $\sigma \geq 2/d$: $\exists\, T^* < \infty$ such that $\lim_{t \to T^*} \|\psi(t)\|_{H^1(\mathbb{R}^d)} = \infty$ ("self-focusing").

Richness of qualitative properties of solutions

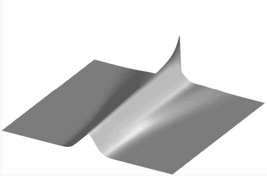
Dispersion : the solution spreads out through space accross time (as in the linear case) : small initial data ψ_0 or small values of nonlinear exponent σ.



Standing wave solutions : nonlinearity is exactly compensated by dispersion effect : solutions propagate in the media with shape invariance.



Blow-up : nonlinearity enforces the solution to focus at one spatial point, either for well-chosen ψ_0 and sufficiently large σ ($\sigma \geq 2/d$) : finite-time blow-up.



Blow-up occurence ?

Predicting finite-time blow-up for solutions of (NLS) considered with an arbitrary Cauchy data ψ_0 in $H^1(\mathbb{R}^d)$ is a delicate question !

However, conditions of blow-up can be derived if $\sigma \geq 2/d$ in terms of the variance $V(t) := \|x\psi\|^2_{L^2(\mathbb{R}^d)}$ if

$$\psi_0 \in \Sigma = \left\{ f \in H^1(\mathbb{R}^d), \quad xf \in L^2(\mathbb{R}^d) \right\}$$

with use of Virial identity (Glassey, Strauss, etc.)

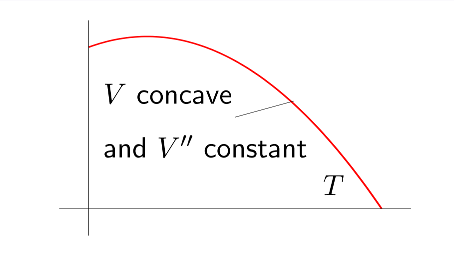
$$\frac{1}{8}\frac{d^2V}{dt^2}(t) = H(\psi_0) + \frac{2 - d\sigma}{2(\sigma+1)} \int_{\mathbb{R}^d} |\psi(t,x)|^{2(\sigma+1)} dx.$$

This enables to give sufficient conditions in the critical $\sigma = 2/d$ and supercritical $\sigma > 2/d$ for a Cauchy data ψ_0 in $H^1(\mathbb{R}^d)$.

Example in the critical case $\sigma = 2/d$

$V''(t) = 8H(\psi_0) = \text{constant} \implies V(t) = 4H(\psi_0)t^2 + \beta t + \gamma.$

Consequently, if $H(\psi_0) < 0$, then $\exists T < \infty$ is such that $V(T) = 0$.

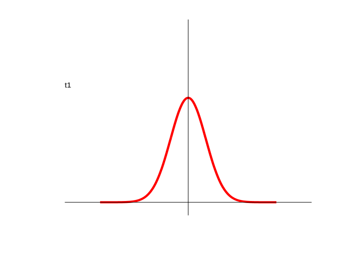


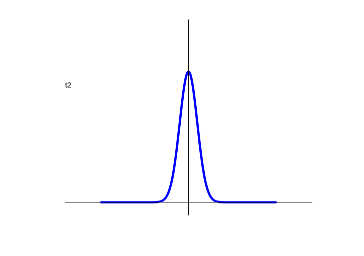
Uncertainty principle : $\|\psi(t)\|^2_{L^2(\mathbb{R}^d)} \leq \frac{2}{d}\sqrt{V(t)}\|\nabla\psi(t)\|_{L^2(\mathbb{R}^d)}$

$$\implies \lim_{t\to T} \|\nabla\psi(t)\|_{L^2(\mathbb{R}^d)} = \infty \text{ and } \lim_{t\to T} \|\psi(t)\|_{H^1(\mathbb{R}^d)} = \infty.$$

Blow-up and scale transition

Finite-time blow-up manifests itself as a transition from large scales to small scales at constant mass.



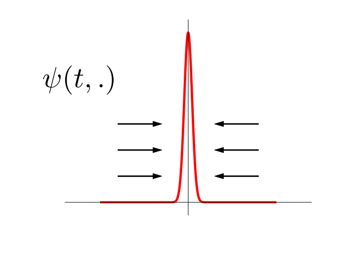


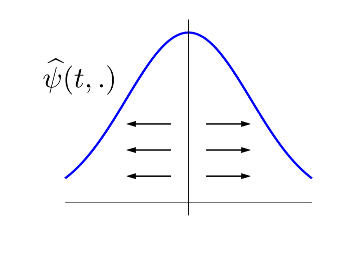
This focusing effect is not related to ordinary differential finite-dimensional collapse :

- $i\partial_t\psi \qquad + |\psi|^{2\sigma}\psi = 0 \implies \psi(t) = \psi_0\, e^{i|\psi_0|^{2\sigma}t}, \quad t \geq 0.$
- $i\partial_t\psi + \Delta\psi \qquad = 0 \implies \|\psi(t)\|_{H^1} = \|\psi_0\|_{H^1},\ t \geq 0.$

Blow-up and scale transition

Finite-time blow-up manifests itself as a transition from large scales to small scales at constant mass.





This focusing effect is not related to ordinary differential finite-dimensional collapse :

- $i\partial_t\psi \qquad\qquad + |\psi|^{2\sigma}\psi = 0 \implies \psi(t) = \psi_0\, e^{i|\psi_0|^{2\sigma} t}, \quad t \geq 0.$
- $i\partial_t\psi + \Delta\psi \qquad\qquad = 0 \implies \|\psi(t)\|_{H^1} = \|\psi_0\|_{H^1}, \; t \geq 0.$

Aim of this study

Possible risks :

- The simplified model may not include realistic dynamics of the physical phenomena.
- Numerical methods may not be adapted when dealing with interactions between large scales and small scales.

Numerical study of a stochastic model :

- Noisy nonlinear optics model involving non-deterministic term that can model inhomogeneities in the media or neglected terms in the initial physical model.
- Influence of the noise term on time-dynamics of stationary and blowing up solutions.

2. Simulation of a stochastic model

$$i\frac{\partial u}{\partial t} + \Delta u + |u|^{2\sigma} u = \varepsilon\, g(u) \quad (\varepsilon \ll 1 \text{ amplitude}).$$

The right-hand *stochastic* term g may involve either neglected terms in the initial governing model (expansion of the index in terms of the field intensity, susceptibility tensor of the nonlinear media) either inhomogeneities of the media.

Possible choices of g :

- $g(u) = \dot{\chi}$ (additive noise) : involves a real white noise both in time and space as a source term.
- $g(u) = \dot{\chi}\, u$ (multiplicative noise) : the white noise acts as a potential term (this matches the L^2 norm conservation for the corresponding solutions).

Noise definition

Let $(\Omega, \mathcal{F}, \mathbb{P})$ a probability space, that consists in Ω (random field space), $\mathcal{F}$ (filtration) and $\mathbb{P}$ (probability on Ω).

If $x \in D$, let $(W(t))_{t\geq 0}$ a real-valued cylindrical Wiener process on $L^2(D)$: for $(e_k)_{k\in\mathbb{N}}$ othonormal basis of $L^2(D)$, then the family $\beta_k(t) := (W(t), e_k)_{L^2(D)}$ defines a family of Brownian motions.

We then have $W(t,x,\omega) = \displaystyle\sum_{k=0}^{\infty} \beta_k(t,\omega) e_k(x),\ x \in D,\ \omega \in \Omega.$

We also set

$$\dot{\chi} := \frac{dW}{dt}(t,x,\omega) = \sum_{k=0}^{\infty} \frac{d\beta_k}{dt}(t,\omega) e_k(x),\ x \in D,\ \omega \in \Omega.$$

This noise term is very irregular both in time and space : its correlation length zero in t and x ! !

What do we want ?

Understand the noise term influence on the dynamics of stationary states and blowing-up solutions that are quite well-known in the deterministic case (that is without noise).

Numerical difficulties :

- Discretization of the (non-smooth) noise term.
- $\psi = \psi(t,x)$ (deterministic) $\longmapsto u = u(t,x,\omega)$ (stochastic)

  From the initial data u_0, we have to compute an infinite number of trajectories for a infinite number of noise realizations ω.

Mean over all the trajectories : expectation of the solution

$$\mathbb{E}\, u(t,x) = \int_\Omega u(t,x,\omega)\, d\mathbb{P}.$$

Numerical scheme (in one space dimension)

Strategy : computation of the solution $u_j^n = u(t_n, x_j)$ at the discrete gridpoints $t_n = n\,\delta t$ and $x_j = jh$ on a time and space mesh, using the following discretization :

Deterministic contribution :

$$i\frac{u_j^{n+1} - u_j^n}{\delta t} + (Lu^{n+1/2})_j + f_j^{n+1/2} u_j^{n+1/2} = 0$$

where L stands for the discretized operator ∂_x^2,

$$f_j^{n+1/2} = \frac{1}{\sigma+1} \frac{|u_j^{n+1}|^{2(\sigma+1)} - |u_j^n|^{2(\sigma+1)}}{|u_j^{n+1}|^2 - |u_j^n|^2}$$

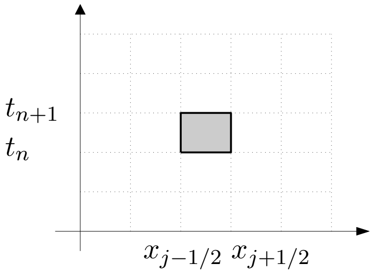
(Crank-Nicolson semi-implicit scheme that mimics at a discrete level mass and energy conservation)

Discretization of the random term :

Equation : $i\partial_t u + \Delta u + |u|^{2\sigma} u = g$

The right-hand term g is discretized with finite volumes, integrating on the elementary cell $]x_{j-1/2}, x_{j+1/2}[\times [t_n, t_{n+1}]$

$$g_j^{n+1/2} \simeq \frac{1}{h\delta t} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{t_n}^{t_{n+1}} g \, ds \, dx.$$



Space domain is discretized in J intervals $I_j =]x_{j-1/2}, x_{j+1/2}[$.

Case of additive noise :

$$\frac{1}{h\,\delta t}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{t_n}^{t_{n+1}} \dot{\chi}\, ds dx = \frac{1}{h\delta t}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{t_n}^{t_{n+1}} \Big(\sum_{k=0}^{\infty} e_k(x) d\beta_k(s)\Big)\, dx$$

$$= \frac{1}{h\,\delta t}\sum_{k=0}^{\infty}\Big(\int_{x_{j-1/2}}^{x_{j+1/2}} e_k(x)\, dx\Big)(\beta_k(t_{n+1}) - \beta_k(t_n)).$$

Choice of basis functions :

We choose the first J functions of the orthonormal basis as indicatrix functions of the J intervals I_j.

$$\Longrightarrow \int_{x_{j-1/2}}^{x_{j+1/2}} e_k(x)\, dx = \sqrt{h}(e_j, e_k)_{L^2(D)} = \sqrt{h}\delta_{j,k}.$$

Hence, source term only involves β_j :

$$g_j^{n+1/2} \simeq \frac{1}{\sqrt{h}}\frac{\beta_j(t_{n+1}) - \beta_j(t_n)}{\delta t}.$$

Case of additive noise :

Discretization of the Brownian term β_k :

$$\theta_j^{n+1/2} = \frac{\beta_j(t_{n+1}) - \beta_j(t_n)}{\sqrt{\delta t}} \sim \mathcal{N}(0,1).$$

Random number generator : $\theta_j^{n+1/2} \longmapsto \chi_j^{n+1/2}$.

$$\Longrightarrow \quad g_j^{n+1/2} \simeq \frac{1}{\sqrt{h\,\delta t}} \chi_j^{n+1/2}.$$

Strategy : this random term is computed on all the gridpoints at each iteration.

Numerically, one has to solve a nonlinear system as in the deterministic case, involving a random contribution in the right-hand term.

Case of multiplicative noise :

Same strategy as or the additive noise and Stratonovitch-like discretization of the stochastic integral

$$\int_{t_n}^{t_{n+1}} u \circ d\beta_j(s) \simeq u\Big(\frac{t_n + t_{n+1}}{2}\Big)\frac{\beta_j(t_{n+1}) - \beta_j(t_n)}{\delta t}.$$

This is compatible with the L^2-norm conservation. This enables to obtain the following discretization of the right-hand term

$$g_j^{n+1/2} = \frac{1}{\sqrt{h\delta t}}\chi_j^{n+1/2}u_j^{n+1/2}.$$

Higher space dimensions :

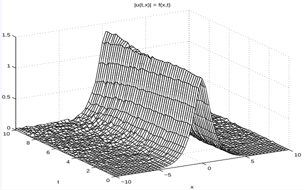
The same arguments will lead us to a multiplicative factor $1/(\sqrt{\delta t}\, h^{d/2})$ if $x \in \mathbb{R}^d$.

3. Numerical results

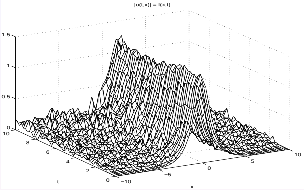
Tasks :

- Numerical investigation of propagation of standing waves solutions in a inhomogeneous nonlinear media : how will the noise affect order of magnitudes of propagation lengths ?
- Study of blow-up occurence arising in the ideal Schrödinger model : could small scales of the noise interfer with focusing effect that is observed in the deterministic case ?

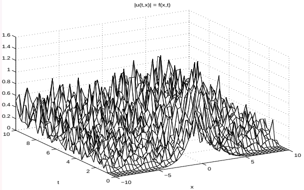
A single example : propagation of a stationary state



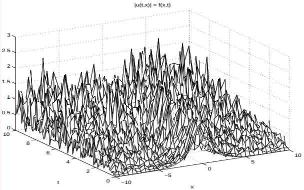
$\varepsilon = 0.01$



$\varepsilon = 0.05$



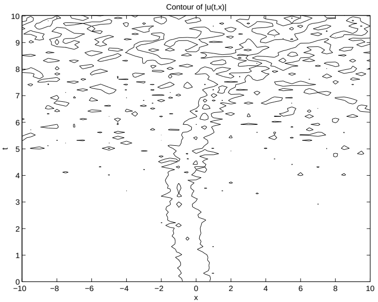
$\varepsilon = 0.2$



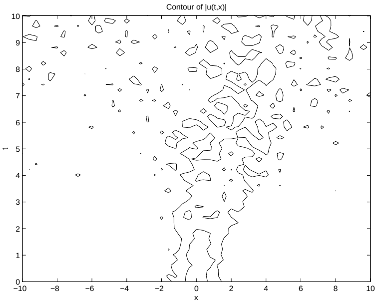
$\varepsilon = 0.5$

A single example : propagation of a stationary state

Propagation of stationary state (explicitly known in dimension 1) : the localized state starts to propagate but is progressively lost due to noise effect. This effect is strong for large noise amplitudes.



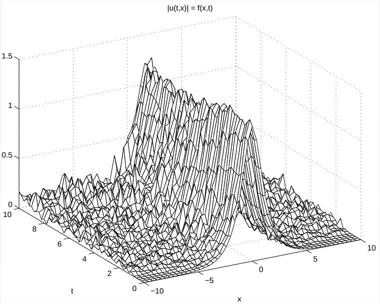
$|u| = |u(t,x,\omega)|$ for a single trajectory, $\varepsilon = 0.2$.



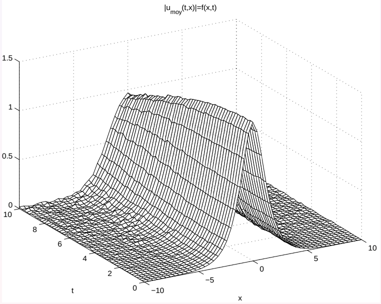
$|u| = |u(t,x,\omega)|$ for a single trajectory, $\varepsilon = 0.5$.

Expectation or trajectory point of view ?

Propagation of stationary state (explicitly known in dimension 1) : persistance of the spatial profile and amplitude attenuation of the expectation (acts as a “soliton diffusion ” effect).

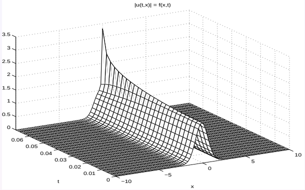


$|u| = |u(t,x,\omega)|$ for a single trajectory ω_0.

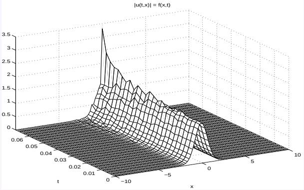


$|\mathbb{E}u| = |\mathbb{E}u(t,x)|$ in the (x,t) plane, (1000 trajectories).

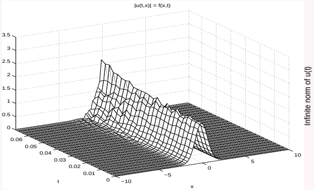
Influence of the noise on blow-up



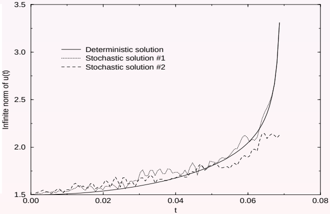
$\varepsilon = 0$



Trajectory $\#1$



Trajectory $\#2$



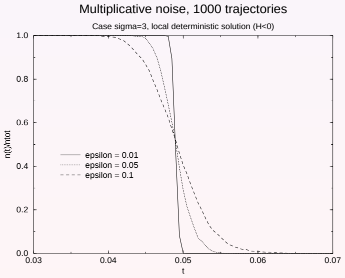
Amplitude plots

Life-time of the trajectories

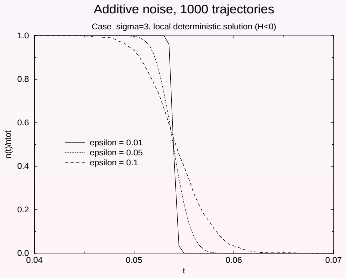
Computation of the quantity $N(t) := \dfrac{n(t)}{N_{tot}}$,

- $n(t)$: number of trajectories still existing at time t ;
- N_{tot} : total number of trajectories.

Blowing-up solutions in the deterministic case :



Multiplicative case



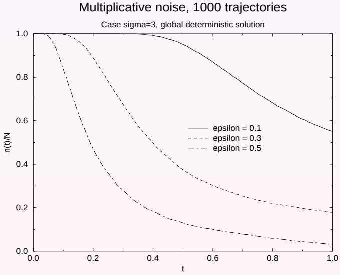
Additive case

Life-time of the trajectories

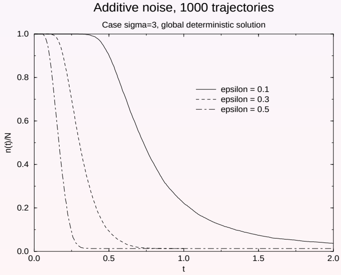
Computation of the quantity $N(t) := \dfrac{n(t)}{N_{tot}}$,

- $n(t)$: number of trajectories still existing at time t ;
- N_{tot} : total number of trajectories.

Global solutions in the deterministic case :



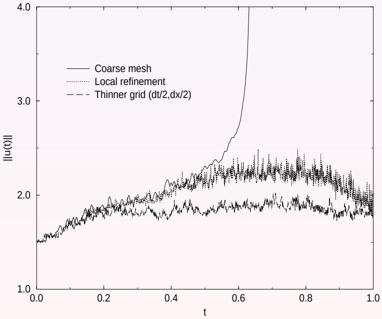
Multiplicative case



Additive case

How to take into account small scales ?

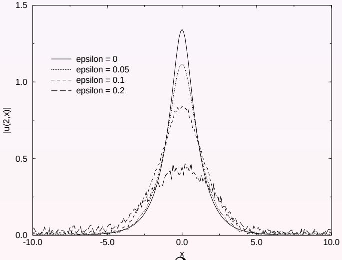
Tests on a uniform grid : irregular noise structure does not manifest when the solution starts to exhibit a blowing-up process $\Longrightarrow$ use of a mesh refinement routine (in order to respect small scales structures of the noise).



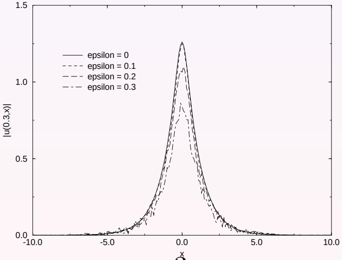
Refinement effect

Numerical observations

- Suppression of blow-up in all the cases, independently of the computed trajectories (consistent with experimentations).
- Soliton diffusion : expectation $\mathbb{E}u$ decreases through times for any σ.



$\sigma = 2$

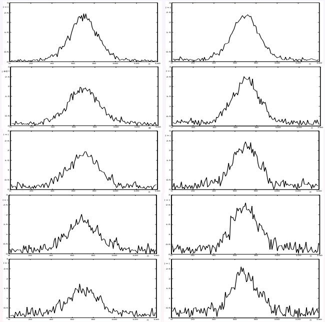


$\sigma = 3$

- Asymptotic law : $\|\mathbb{E}(u(t))\|_{L^\infty(\mathbb{R})} \sim t^{-1}$.

Two-dimensional tests

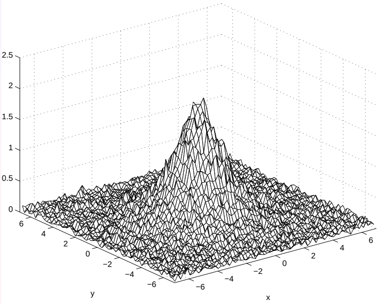
The same behaviour can be observed in the multiplicative case.



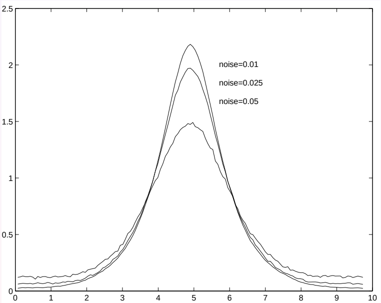
Trace of the solution amplitude at $x_2 = 0$ at times $t = 2,\ 4,\ 6,\ 8,\ 10$, multiplicative case (left) and additive case (right), ($\sigma = \frac{1}{2}$, $\varepsilon = 0.03$)

Soliton diffusion

Propagation of stationary state (computed using the shooting method in dimension 2) in the critical case $\sigma = 1$.



$|u| = |u(t,x,\omega)|$ for a single trajectory ω_0, $\varepsilon = 0.025$.

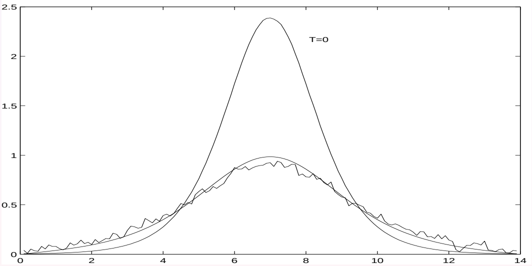


Soliton diffusion for the expectation of the solution.

Numerical observations

Noise diffusion effect can be compared with the one in the Complex Ginzburg-Landau equation (CGL).

$$\frac{\partial u}{\partial t} - (\mu + i)\Delta u + (\nu - i)|u|^{2\sigma} u = 0.$$



Comparison between $\mathbb{E}u$ and the solution of (CGL) at final time T, 2 space dimension, $\mu = \nu = 0.055$, $\sigma = 1$.

What about the computations ?

- For one single noise simulation : one has to solve successive non-linear systems on a spatial grid with a mesh refinement routine (linked to the numerical scheme).
- Given a single Cauchy data, one needs to perform computations with *several thousands* of different trajectories to get relevant information on the solution dynamics (linked to the stochastic aspect of the model).
- For any nonlinearity, one has to solve the nonlinear PDE for many initial data (linked to the nonlinear deterministic part of the model).

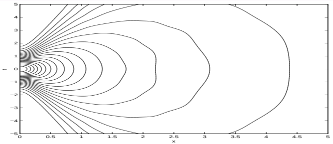
$\Longrightarrow$ Costly computations (many billions of “elementary” resolutions for many trajectories) that easily tolerate parallel computing (all the resolutions are independent).

Possible extensions

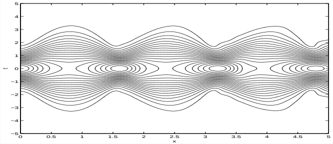
- Equation involving a trapping potential :

$$i\frac{\partial \psi}{\partial t} + \Delta\psi \; - \|x\|^2\psi + |\psi|^{2\sigma}\psi = 0$$

Well-known model to govern the time evolution of a Bose-Einstein condensate at low temperature. Confining potential : enhances space localization even in the linear case !



$i\partial_t\psi = -\Delta\psi.$



$i\partial_t\psi = (-\Delta + \|x\|^2)\psi.$

- Many other possible models that admit explosive and stationary states (wave equations, KdV equations, etc.)