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Waves: propagation, dispersion and numerical simulation

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THE GENERAL PROBLEM:

TO BUILD CONVERGENT NUMERICAL SCHEMES FOR LINEAR/NONLINEAR PARTIAL DIFFERENTIAL EQUATIONS (PDE).

To reproduce in the computer the dynamics in Continuum and Quantum Mechanics, avoiding spurious numerical solutions.

WARNING!

NUMERICS = CONTINUUM + (POSSIBLY) SPURIOUS

In this talk we address two examples:

Example 1: NONLINEAR SCHRÖDINGER EQUATION.

Similar problems for other dispersive equations: Korteweg-de-Vries, wave equation, ...

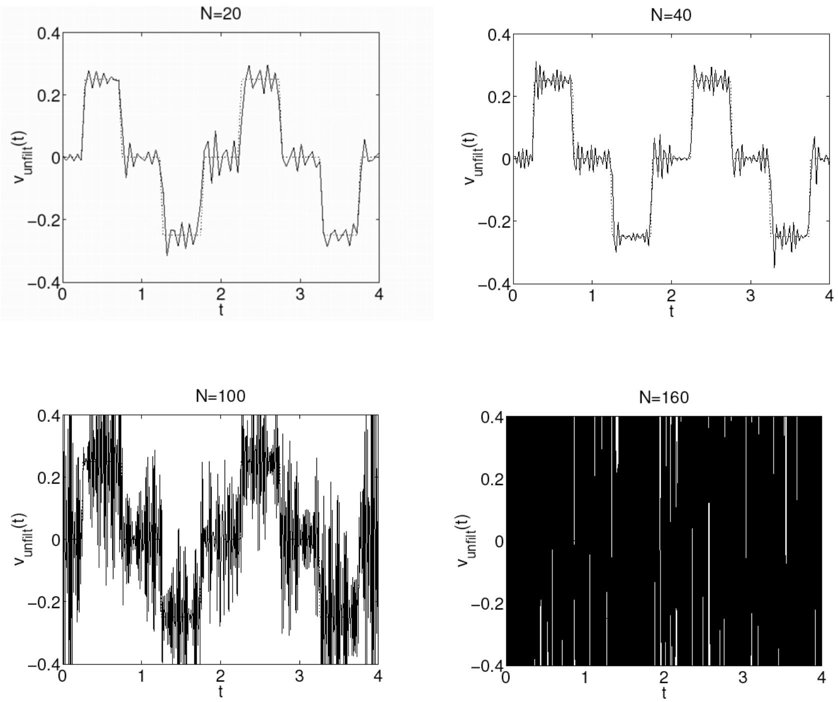
Example 2: MULTI-STRUCTURES.

Ton capture the fine hidden properties of interaction in multi-body or multi-linked structures.

MESSAGE: Classical numerical analysis requires of added important developments in order to be in conditions of covering complex systems of PDE arising in Sciences and Technologies. In particular, fine tools of Harmonic analysis have to be developed.

FROM FINITE TO INFINITE DIMENSIONS IN PURELY CONSERVATIVE SYSTEMS.....

E. Z. SIAM Review, 47 (2) (2005), 197-243.



PRELIMINARIES

Most of what is currently done in the numerical analysis of nonlinear PDE is based on the following ingredients:

1.- Well-posedness of the underlying continuous linear problem:

$$\frac{du}{dt}(t) = Au(t), \quad t \geq 0; \quad u(0) = u_0.$$

The solution is given by $u(t) = e^{At}u_0$ and lies in $C([0,T];H)$, H being the natural "energy space" (Hilbert or Banach).

Semigroup theory provides a rigorous justification of this provided A is *maximal-dissipative* ($A \leq 0$).

Most of the *linear* PDE from Mechanics enter in this general frame: wave, heat, Schrödinger equations,...

2.- Nonlinear problems are solved by using *fixed point arguments* on the *variation of constants formulation* of the PDE:

$$u_t(t) = Au(t) + f(u(t)), \quad t \geq 0; \quad u(0) = u_0.$$

$$u(t) = e^{At}u_0 + \int_0^t e^{A(t-s)} f(u(s))ds.$$

Assuming !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!! $f : H \to H$ is locally Lipschitz, allows proving local (in time) existence and uniqueness in

$$u \in C([0, T]; H).$$

But, often in applications, the property that $f : H \to H$ is locally Lipschitz FAILS.

For instance $H = L^2(\Omega)$ and $f(u) = |u|^{p-1}u$, with $p > 1$.

Inverse and control problems often do not find a natural answer in the same functional setting. H, which is built for solving the Cauchy problem, might not be the right space for other problems.

3.- To avoid this difficulty it is convenient to work on spaces

$$C([0,T];H) \cap X,$$

X being "adapted" to the system (the linear flow is stable in X): e^{At} maps X into itself.

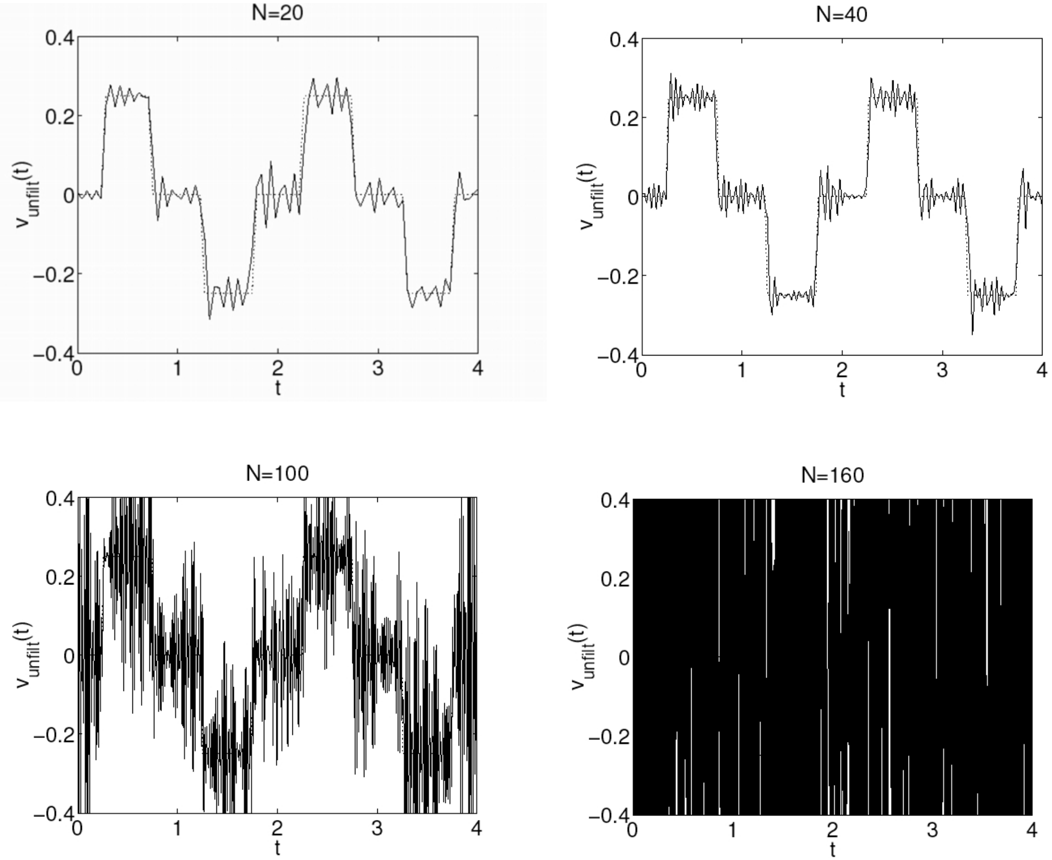
This allows testing the Lipschitz properties of the nonlinearity f in the smaller space $C([0,T];H) \cap X$.

Typically in applications $X = L^r(0,T;L^q(\Omega))$. This allows enlarging the class of solvable nonlinear PDE in a significant way.

4.- BUT, in order to prove convergence of numerical methods, it is then needed:

- To check consistency and stability in H. This gurantees convergence in the classical energy space according to Lax' equivalence criterium;

- To check stability in X as well. This may be difficult in practice and standard numerical algorithms often fail to have that property.

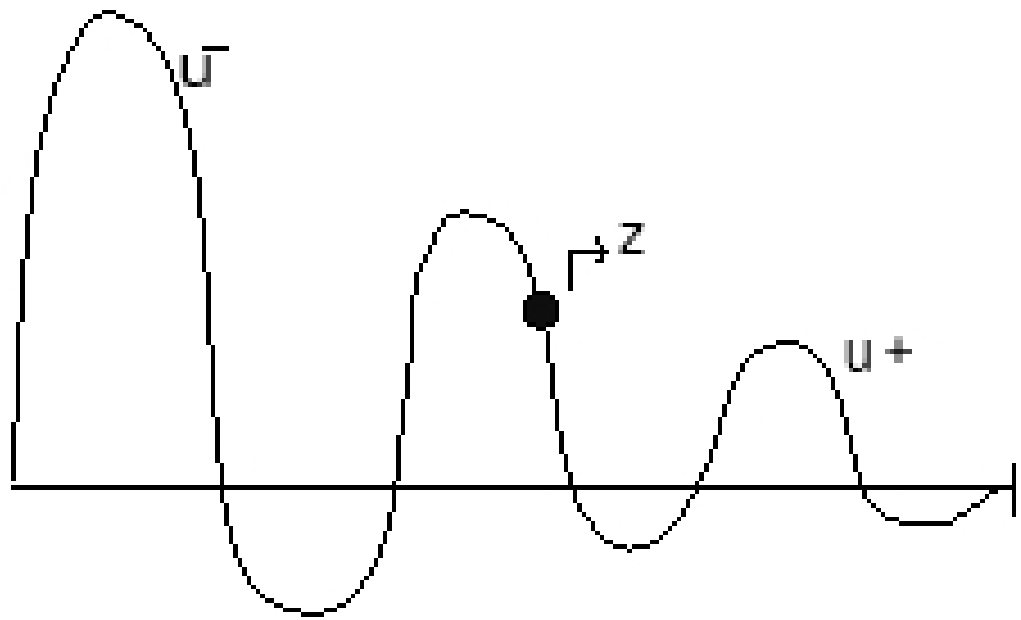


A convergent numerical scheme (in H) that fails to reproduce some other dynamical properties (in X)(boundary control of waves).

VIBRATIONS OF MULTI-D STRUCTURES: $0-D+1-D$

(S. Hansen & E. Z, 1995, C. Castro & E. Z., 1996)

string+point mass + string



u⁻
z
u+

$$
\begin{cases}
u^-_{tt} - u^-_{xx} = 0, & -1 < x < 0, \quad t > 0 \\
u^+_{tt} - u^+_{xx} = 0, & 0 < x < 1, \quad t > 0 \\
z''(t) = \left[u^+_x(0,\, t) - u^-_x(0,\, t)\right], & t > 0 \\
z(t) = u^-(0,\, t) = u^+(0,\, t), & t > 0 \\
u^-(-1,\, t) = u^+(1,\, t) = 0, & t > 0 \\
+ \text{ initial conditions} &
\end{cases}
$$

The energy of the system is conserved:

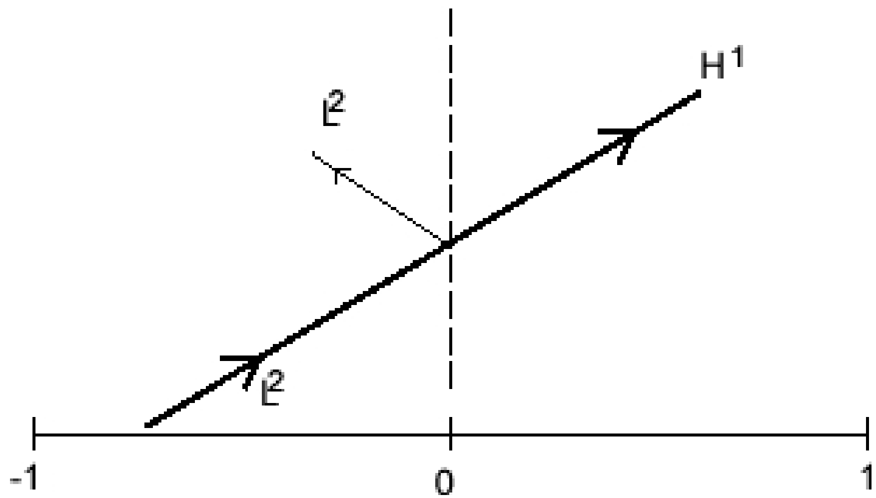
$$E(t) = E_-(t) + E_+(t) + E_m(t)$$
$$E_- = \frac{1}{2}\int_{-1}^{0} \left[\mid u_t^- \mid^2 + \mid u_x^- \mid^2\right] dx$$
$$E_+ = \frac{1}{2}\int_{0}^{1} \left[\mid u_t^+ \mid^2 + \mid u_x^+ \mid^2\right] dx$$
$$E_m = \frac{1}{2} \mid z' \mid^2 = \frac{1}{2} \left|\frac{dz}{dt}\right|^2 .$$

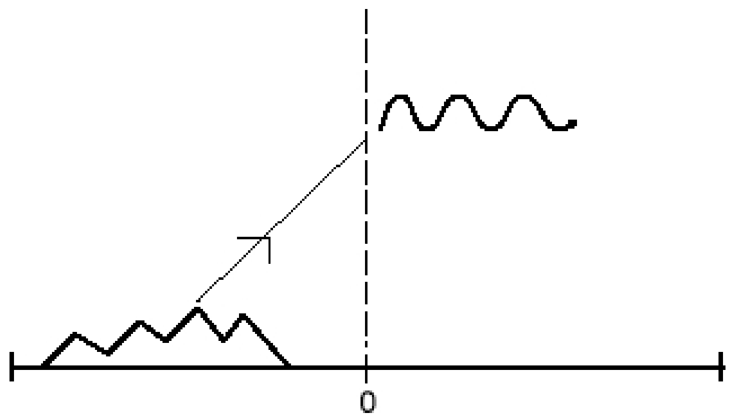
Accordingly the system is welposed in the energy space:

$$H = H_0^1(-1, 1) \times L^2(-1, 1) \times \mathbb{R}$$

This can be seen by all standard methods: semigroups, Galerkin,...

A careful (but simple) analysis of the propagation of waves when crossing the point-mass (using d'Alembert's formula) shows that a unexpected property holds: Waves are regularized by one derivative when crossing the mass.





As a consequence of this fact: The system is well-posed in an asymmetric space: finite energy solutions to one side, plus, one more derivative in L^2 in the other one:

$$\left[H^1(-1,0)\times L^2(-1,0)\right]\times\left[H^2(0,1)\times H^1(0,1)\right].$$

OF COURSE, THIS PROPERTY IS NOT TRUE FOR THE CLASSICAL CONSTANT COEFFICIENT WAVE EQUATION BECAUSE OF THE PROPAGATION OF SINGULARITIES.

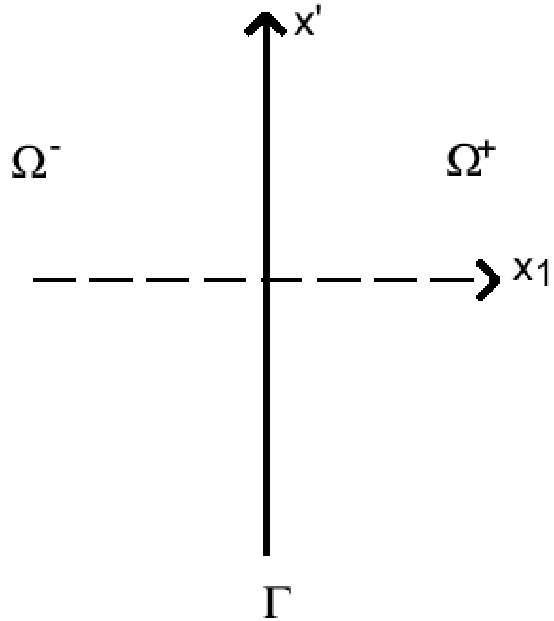
These properties have also important consequences in what concerns the control and inverse problems. The observations, and action of controllers have to cross the point mass, making the natural spaces for these problems to be asymmetric.

- Can this atypical asymmetric well-posedness property be predicted by classical methods?

- Are there numerical algorithms that reproduce asymmetry?

EXTENSION TO $2-D$

(H. Koch & E. Z., 2005)



$$\begin{cases} u^-_{tt} - \Delta u^- = 0 & \Omega^- \times (0, \infty) \\ v_{tt} - c^2 \Delta' v = [u_{x_1}] & \Gamma \times (0, \infty) \\ u^+_{tt} - \Delta u^+ = 0 & \Omega^+ \times (0, \infty) \end{cases}$$

The energy

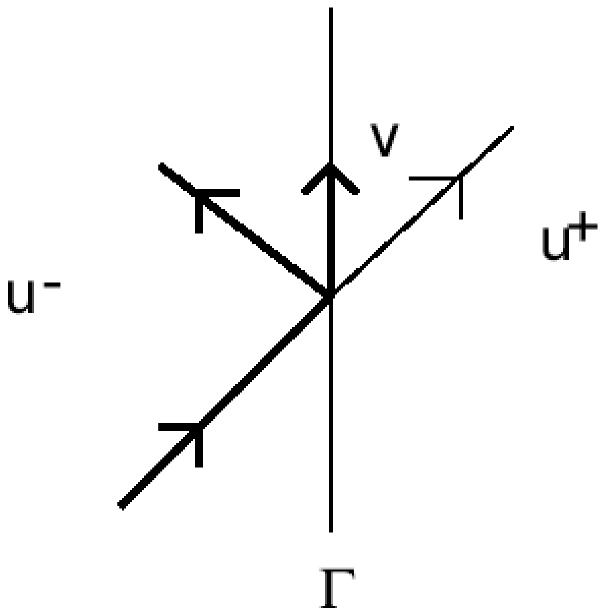
$$E(t) = \frac{1}{2}\int_{\Omega^-} \left(| u^-_t |^2 + | \nabla u^- |^2\right) dx + \frac{1}{2}\int_{\Omega^+} \left(| u^+_t |^2 + | \nabla u^+ |^2\right) dx$$
$$+ \frac{1}{2}\int_{\Gamma} \left(| v_t |^2 + | \nabla' v |^2\right) dx'$$

is constant in time and the system is well-posed in the natural energy space.

$$\left[H^1(\Omega^-) \times L^2(\Omega^-)\right] \times \left[H^1(\Gamma) \times L^2(\Gamma)\right] \times \left[H^1(\Omega^+) \times L^2(\Omega^+)\right]$$

IS THE SYSTEM WELL-POSED IN ANY ASYMMETRIC SPACE?

PLANE WAVE ANALYSIS ALLOWS EXCLUDING THIS PROPERTY IN A NUMBER OF SITUATIONS



THE GENERAL PRINCIPLE:

Incoming waves $\rightarrow$ reflected wave+ wave absorbed by the interface.+transmission wave.

$$\begin{aligned} u^- &= e^{i(x\cdot\xi+\tau t)/\varepsilon} + ae^{i(x\cdot\tilde{\xi}+\tau t)/\varepsilon} = \text{incoming} + \text{reflected wave} \\ u^+ &= be^{i(x\cdot\xi+\tau t)/\varepsilon} = \text{ transmission wave} \\ v &= be^{i(x'\cdot\xi'+\tau t)/\varepsilon} = \text{absorbed wave} \end{aligned}$$

$$\xi = (\xi_1, \xi'); \tilde{\xi} = (-\xi_1, \xi'); \tau^2 = |\ \xi\ |^2 .$$

$a =$ reflection coefficient.

$b =$ transmission coefficient = absorption coefficient.

Continuity condition on the interface:

$$1 + a = b$$

Note that the restriction of all waves to the interface $x_1 = 0$ is an oscillatory tangential wave of the form $e^{i(x'\cdot\xi'+\tau t)/\varepsilon}$ up to a constant multiplicative factor.

$$\Box_c' v = \left(\partial_t^2 - c^2 \Delta'\right) v = -\frac{b}{\varepsilon^2}\left(\tau^2 - c^2 \mid \xi' \mid^2\right) e^{i(x'\xi' + \tau t)/\varepsilon}$$

$$[u_{x_1}] = u_{x_1}^{+} - u_{x_1}^{-} = \frac{2a\xi_1 i}{\varepsilon} e^{i(x'\xi' + \tau t)/\varepsilon}$$

Consequently, in view of the equation $v_{tt} - c^2\Delta' v = [u_{x_1}]$, and the fact that $\tau^2 = |\xi_1|^2 + |\xi'|^2$,

$$-\frac{b}{\varepsilon^2}\left(\tau^2 - c^2 \mid \xi' \mid^2\right) = -\frac{b}{\varepsilon^2}\left(\xi_1^2 + (1 - c^2) \mid \xi' \mid^2\right) = \frac{2a\xi_1 i}{\varepsilon}$$

$$a = -\frac{\xi_1^2 + (1 - c^2) \mid \xi' \mid^2}{2i\varepsilon\xi_1 + \left(\xi_1^2 + (1 - c^2) \mid \xi' \mid^2\right)}$$

$$b = \frac{2i\varepsilon\xi_1}{2i\varepsilon\xi_1 + \xi_1^2 + (1 - c^2) \mid \xi' \mid^2}$$

THREE CASES

$\boxed{c = 1}$

$$b = \frac{2i\varepsilon}{\xi_1 + 2i\varepsilon}$$

$$\xi_1 \sim \varepsilon \Rightarrow b \sim \frac{2i}{1 + 2i}$$

EFFECTIVE TRANSMISSION.

THIS IS INCOMPATIBLE WITH WELL-POSEDNESS IN ASYMMETRIC SPACES

$\boxed{c < 1}$

$$\xi_1^2 + (1 - c^2) \mid \xi' \mid^2 \geqslant \alpha \mid \xi \mid^2$$

$$b = \frac{2i\varepsilon\xi_1}{2i\varepsilon\xi_1 + \xi_1^2 + (1 - c^2) \mid \xi' \mid^2} \sim \varepsilon \to 0.$$

NO TRANSMISSION.

COMPATIBLE WITH WELL-POSEDNESS IN ASYMMETRIC SPACES.

$c > 1$

In this case there are directions in which the quadratic denominator of the formulas we found vanishes.

$$\xi_1^2 + (1 - c^2) \mid \xi' \mid^2 = 0$$

$$\mid \xi_1 \mid = \sqrt{\frac{c^2 - 1}{1 + c^2}}$$

In that direction

$$b = 1$$

COMPLETE TRANSMISSION.

INCOMPATIBLE WITH WELL-POSEDNESS IN ASYMMETRIC SPACES

Theorem (H. Koch & E. Z., 2005):

- The problem may not be well-posed in asymmetric spaces when $c \geqslant 1$.

- The problem is indeed well-posed in asymmetric spaces when $c < 1$:

$$\underbrace{H^1(\Omega^-) \times L^2(\Omega^-)}_{u^-} \times \underbrace{H^2(\Gamma) \times H^1(\Gamma)}_{v} \times \underbrace{H^2(\Omega^+) \times H^1(\Omega^+)}_{u^+}$$

PROOF: The negative result is a consequence of the plane wave analysis above. The positive one requires of a more careful microlocal analysis.

FINITE DIFFERENCE APPROXIMATIONS

IN $1-d$ THE STANDARD FINITE-DIFFERENCE SEMIDISCRETIZATION SCHEME CONVERGES IN THE CLASSICAL ENERGY SPACE BUT ALSO IN THE SHARP ASYMMETRIC SPACES.

Energy methods yield finite energy solutions in $H^1_{x,t}$.

Hidden regularity for solutions of the wave equation $\rightarrow \partial_x u^{\pm}(0,t) \in L^2_t$.

The interface equation $z''(t) = \left[u_x^+(0,\, t) - u_x^-(0,\, t)\right]$

The Dirichlet boundary data for the wave equations in $x < 0$ and $x > 0$, z, lie in H^2_t.

Consequently, $u^- \in H^1_{x,t}$ and $u^+ \in H^2_{x,t}$, as solutions of their corresponding non-homogeneous boundary value problems.

THE SAME ARGUMENTS APPLY FOR THE NUMERICAL SCHEME, UNIFORMLY ON THE MESH-SIZE.

OPEN PROBLEMS:

CHECK IF THE SAME IS TRUE IN SEVERAL SPACE DIMENSIONS.

BUILD NUMERICAL METHODS THAT CONVERGE IN ASYMMETRIC SPACES.

NOTE THAT STANDARD ENERGY METHODS DO NOT SUFFICE!

DIFFERENT MESHES ON THE VARIOUS COMPONENTS/DOMAINS OF THE SYSTEM?

DOMAIN DECOMPOSITION TECHNIQUES....

THE NONLINEAR SCHRÖDINGER EQUATION

Work in collaboration with Liviu Ignat, C. R. Acad. Sci. Paris, **340** (7) (2005), 529534.

Key point: To handle nonlinearities one needs to decode the intrinsic hidden properties of the underlying linear differential operators (Strichartz, Bourgain, Kenig, Ponce, Saut, Vega, Burq, Gérard, ...)

This has been done succesfully for the PDE models.

What about Numerical schemes?

The Linear Schrödinger Equation (LSE):

$$\begin{cases} iu_t + u_{xx} = 0 & x \in \mathbf{R}, t > 0, \\ u(0,x) = \varphi & x \in \mathbf{R}. \end{cases} \tag{1}$$

It may be written in the abstract form:

$$u_t = Au,$$

with

$$A = i\Delta = i\partial^2 \cdot /\partial x^2.$$

Accordingly, the LSE generates a group of isometries $e^{i\Delta t}$ in $L^2(\mathbf{R})$, i. e.

$$||u(t)||_{L^2(\mathbf{R})} = ||\varphi||_{L^2(\mathbf{R})}, \quad \forall t \geq 0.$$

The fundamental solution is explicit $G(x,t) = (4i\pi t)^{-1/2}\exp(-|x|^2/4i\pi t)$.

Dispersive properties: Fourier components with different wave numbers propagate with different velocities.

- $L^1 \to L^\infty$ decay.

$$||u(t)||_{L^\infty(\mathbf{R})} \le (4\pi t)^{-\frac{1}{2}} ||\varphi||_{L^1(\mathbf{R})}.$$

$$||u(t)||_{L^p(\mathbf{R})} \le (4\pi t)^{-(\frac{1}{2}-\frac{1}{p})} ||\varphi||_{L^{p'}(\mathbf{R})}, 2 \le p \le \infty.$$

- Local gain of 1/2-derivative: If the initial datum φ is in $L^2(\mathbf{R})$, then $u(t)$ belongs to $H^{1/2}_{loc}(\mathbf{R})$ for a.e. $t \in \mathbf{R}$.

These properties are not only relevant for a better understanding of the dynamics of the linear system but also to derive well-posedness results for nonlinear Schrödinger equations (NLS).

The classical three-point finite-difference scheme

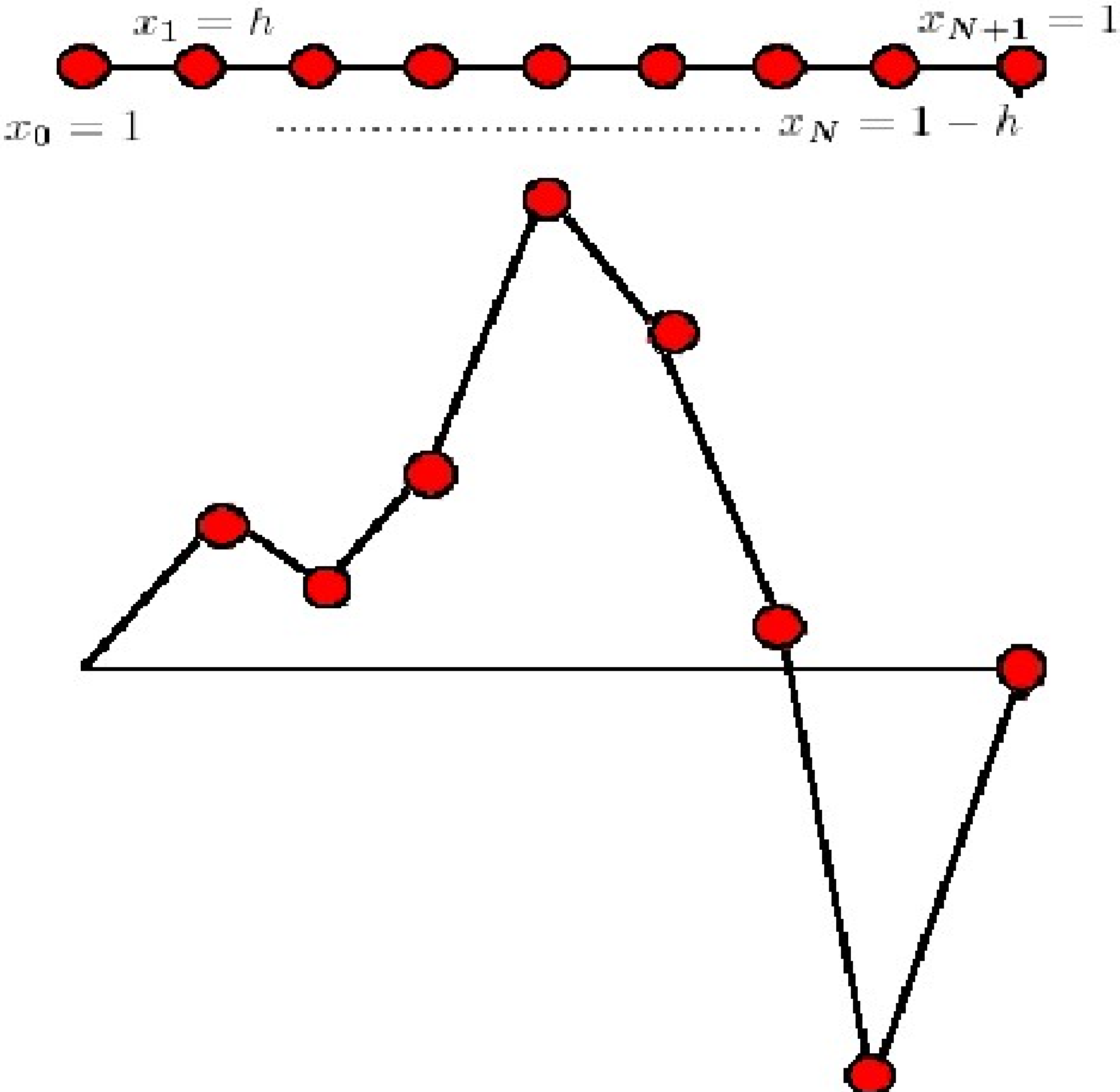
Consider the finite difference approximation

$$i\frac{du^h}{dt} + \Delta_h u^h = 0, t \neq 0, \quad u^h(0) = \varphi^h. \tag{2}$$

Here $u^h \equiv \{u_j^h\}_{j\in\mathbf{Z}}$, $u_j(t)$ being the approximation of the solution at the node $x_j = jh$, and $\Delta_h \sim \partial_x^2$:

$$\Delta_h u = \frac{1}{h^2}[u_{j+1} + u_{j-1} - 2u_j].$$

The scheme is consistent + stable in $L^2(\mathbf{R})$ and, accordingly, it is also convergent, of order 2 (the error is of order $O(h^2)$).



$x_1 = h$
$x_{N+1} = 1$
$x_0 = 1$
$x_N = 1 - h$

In fact,

$$||u^h(t)||_{\ell^2} = ||\varphi||_{\ell^2},$$

for all $t \geq 0$.

The same convergence result holds for semilinear equations provided the nonlinearity $f : \mathbf{R} \to \mathbf{R}$ is globally Lipschitz.

BUT THIS ANALYSIS IS INSUFFICIENT TO DEAL WITH OTHER NONLINEARITIES, FOR INSTANCE:

$$f(u) = |u|^{p-1}u, \quad p > 1.$$

IT IS JUST A MATTER OF WORKING HARDER, OR DO WE NEED TO CHANGE THE NUMERICAL SCHEME?

LACK OF DISPERSION OF THE NUMERICAL SCHEME

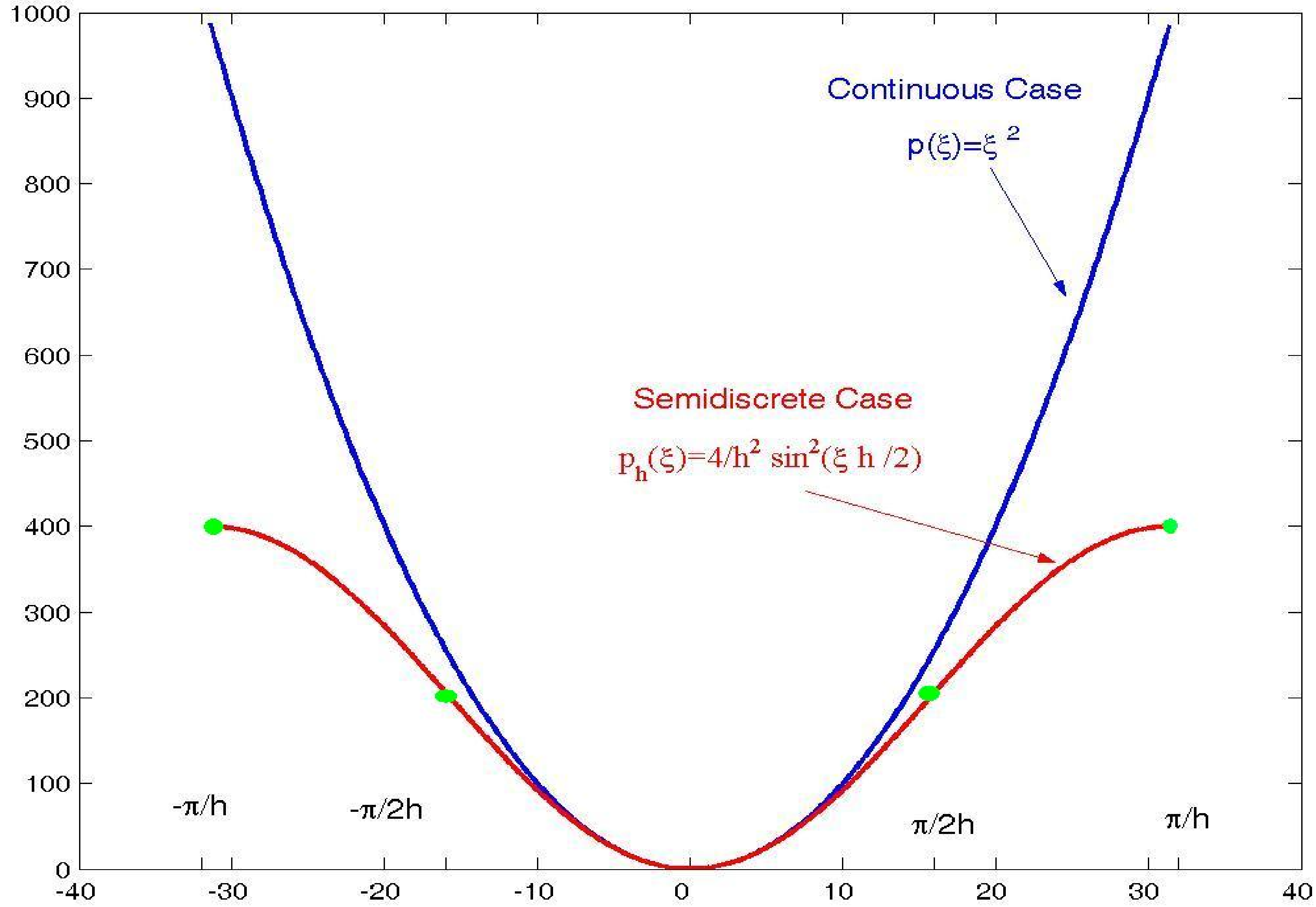
Consider the semi-discrete Fourier Transform

$$\hat{u} = h \sum_{j \in \mathbf{Z}} u_j e^{-ijh\xi}, \quad \xi \in [-\frac{\pi}{h}, \frac{\pi}{h}].$$

There are "slight" but important differences between the symbols of the operators Δ and Δ_h:

$$p(\xi) = -\xi^2, \xi \in \mathbf{R}; \quad p_h(\xi) = -\frac{4}{h^2} \sin^2(\frac{\xi h}{2}), \xi \in [-\frac{\pi}{h}, \frac{\pi}{h}].$$

For a fixed frequency ξ, obviously, $p_h(\xi) \to p(\xi)$, as $h \to 0$. This confirms the convergence of the scheme. But this is far from being sufficient for oul goals.


Continuous Case
p(ξ)=ξ 2
Semidiscrete Case
p_h(ξ)=4/h² sin²(ξ h /2)
-π/h
-π/2h
π/2h
π/h
1000
900
800
700
600
500
400
300
200
100
0
-40
-30
-20
-10
0
10
20
30
40

The main differences are:

- $p(\xi)$ is a convex function;

  $p_h(\xi)$ changes the convexity at $\pm\frac{\pi}{2h}$.

- $p'(\xi)$ has a unique zero, $\xi = 0$;

  $p'_h(\xi)$ has the zeros at $\xi = \pm\frac{\pi}{h}$ as well.

These "slight" changes on the shape of the symbol are not an obstacle for the convergence of the numerical scheme in the $L^2(\mathbf{R})$ sense. But produce the lack of uniform (in h) dispersion.

LACK OF CONVEXITY = LACK OF INTEGRABILITY GAIN.

The symbol $p_h(\xi)$ looses convexity near $\pm\pi/2h$. Applying the stationary phase lemma (T. Carbery, G. Gigante, F. Soria):

Theorem 1 *Let $1 \leq q_1 < q_2$. Then, for all positive t,*

$$\sup_{h>0, \varphi^h \in l_h^{q_1}(\mathbf{Z})} \frac{|| \exp(it\Delta_h)\varphi^h ||_{l_h^{q_2}(\mathbf{Z})}}{||\varphi^h||_{l_h^{q_1}(\mathbf{Z})}} = \infty. \quad (3)$$

Initial datum with Fourier transform concentrated on $\pi/2h$.

LACK OF CONVEXITY = LACK OF LAPLACIAN.

A. Stefanov & P. G. Kevrekidis, Nonlinearity 18 (2005) 1841–1857.

The fundamental solution of the numerical problem decays as $t^{-1/3}$ and not $t^{-1/2}$.

Lemma 1 *(Van der Corput)*

Suppose ϕ is a real-valued and smooth function in (a, b) that $|\phi^{(k)}(\xi)| \geq 1$ for all $x \in (a, b)$. Then

$$\left| \int_a^b e^{it\phi(\xi)} d\xi \right| \leq c_k t^{-1/k} \tag{4}$$

LACK OF SLOPE= LACK OF REGULARITY GAIN.

Theorem 2 *Let $q \in [1,2]$ and $s > 0$. Then*

$$\sup_{h>0, \varphi^h \in l_h^q(\mathbf{Z})} \frac{\left| S^h(t)\varphi^h \right|_{\hbar^s_{loc}(\mathbf{Z})}}{\left| \varphi^h \right|_{l_h^q(\mathbf{Z})}} = \infty. \tag{5}$$

Initial data whose Fourier transform is concentrated around π/h.

LACK OF SLOPE= VANISHING GROUP VELOCITY.

Trefethen, L. N. (1982). SIAM Rev., **24** *(2), pp. 113–136.*

A REMEDY: FOURIER FILTERING *Eliminate the pathologies that are concentrated on the points* $\pm\pi/2h$ *and* $\pm\pi/h$ *of the spectrum.*

Replace the complete solution

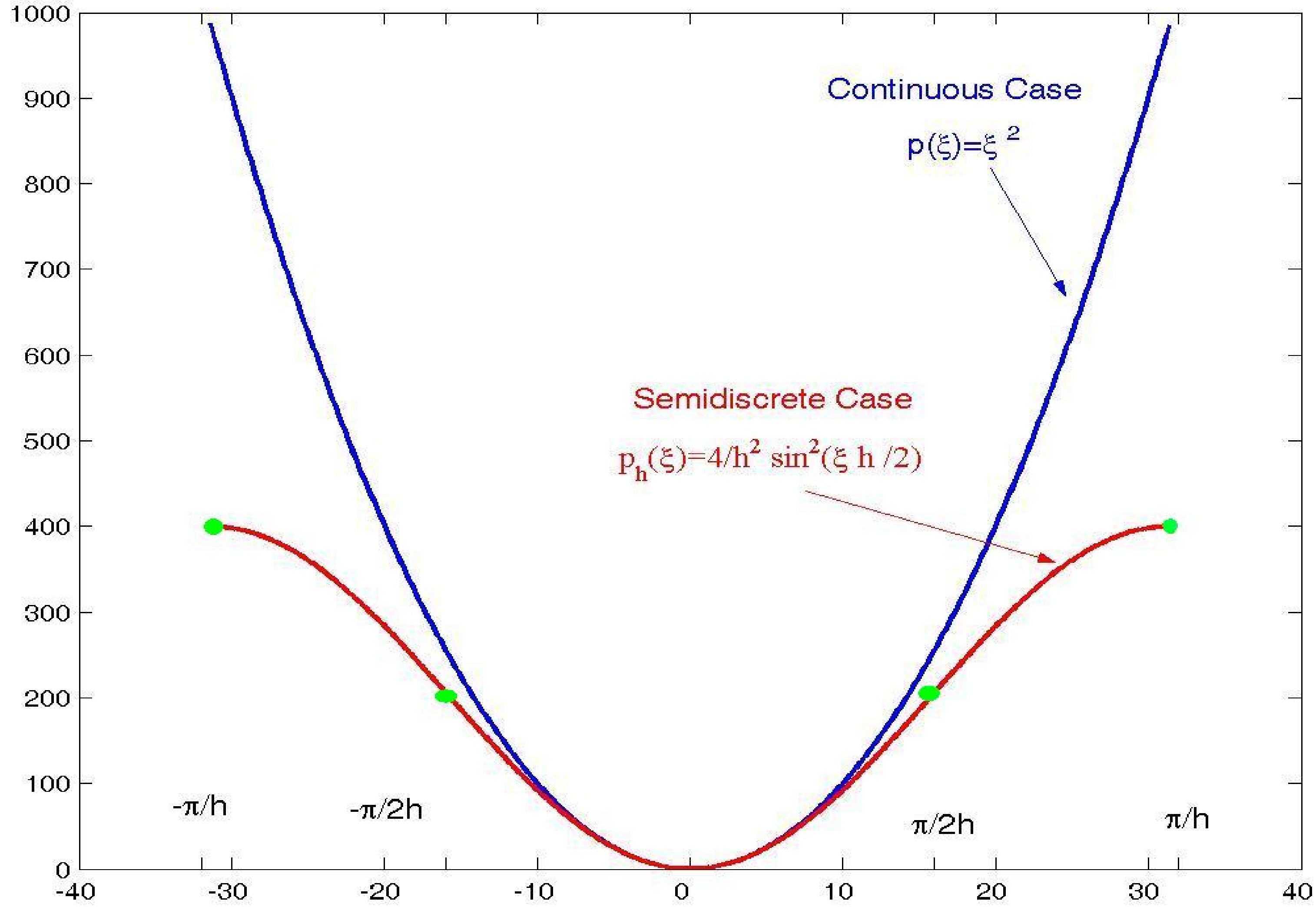
$$u_j(t) = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} e^{ijh\xi} e^{ip_h(\xi)t} \hat{\varphi}(\xi)d\xi, \quad j \in \mathbf{Z}.$$

by the filtered one

$$u_j^*(t) = \frac{1}{2\pi}\int_{-(1-\delta)\pi/2h}^{(1-\delta)\pi/2h} e^{ijh\xi} e^{ip_h(\xi)t} \hat{\varphi}(\xi)d\xi, \quad j \in \mathbf{Z}.$$

a) This guarantees the same dispersion properties of the continuous Schrödinger equation to be uniformly (on h) true;

b) The convergence of the filtered numerical scheme still holds.



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But Fourier filtering:

- *Is computationally expensive: Compute the complete solution in the numerical mesh, compute its Fourier tranform, filter and the go back to the physical space by applying the inverse Fourier transform;*

- *Is of little use in nonlinear problems.*

Other more efficient methods?

A VISCOUS FINITE-DIFFERENCE SCHEME

Consider:

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h &= ia(h)\Delta_h u^h, \quad t > 0, \\ u^h(0) &= \varphi^h, \end{cases} \tag{6}$$

where the numerical viscosity parameter $a(h) > 0$ is such that

$$a(h) \to 0$$

as $h \to 0$.

This condition guarantess the consistency.

This scheme generates a dissipative semigroup $S_+^h(t)$, for $t > 0$:

$$||u(t)||_{\ell^2}^2 = ||\varphi||_{\ell^2}^2 - 2a(h)\int_0^t ||u(\tau)||_{\hbar^1}^2 d\tau.$$

Two dynamical systems are mixed in this scheme:

- *the purely conservative one,* $i\frac{du^h}{dt} + \Delta_h u^h = 0$,
- *the heat equation* $u_t^h - a(h)\Delta_h u^h = 0$ *with viscosity* $a(h)$.

Viscous regularization is a typical mechanism to improve convergence of numerical schemes: hyperbolic conservation laws and shocks, level set methods for image processing, ...

The receipt:

"Convergent numerical scheme + extra viscosity (at a suitable scale), keeps convergence and enhances the regulartity of solutions and the stability of the scheme".

The main dispersive properties of this scheme are as follows:

Theorem 3 *(L^p-decay) Let fix $p \in [2, \infty]$ and $\alpha \in (1/2, 1]$. Then for*

$$a(h) = h^{2-1/\alpha},$$

$S_{\pm}^h(t)$ maps continuously $l_h^{p'}(\mathbf{Z})$ to $l_h^p(\mathbf{Z})$ and there exists some positive constants $c(p)$ such that

$$||S_{\pm}^h(t)\varphi^h||_{l_h^p(\mathbf{Z})} \leq c(p)(|t|^{-\alpha(1-\frac{2}{p})} + |t|^{-\frac{1}{2}(1-\frac{2}{p})})||\varphi^h||_{l_h^{p'}(\mathbf{Z})} \tag{7}$$

holds for all $|t| \neq 0$, $\varphi \in l_h^{p'}(\mathbf{Z})$ and $h > 0$.

Theorem 4 *(Smoothing) Let* $q \in [2\alpha, 2]$ *and* $s \in [0, 1/2\alpha - 1/q]$*. Then for any bounded interval* I *and* $\psi \in C_c^\infty(\mathbf{R})$ *there exists a constant* $C(I, \psi, q, s)$ *such that*

$$\left|\psi E^h u^h(t)\right|_{L^2(I;H^s(\mathbf{R}))} \leq C(I, \psi, q, s) \left|\varphi^h\right|_{l_h^q(\mathbf{Z})}. \tag{8}$$

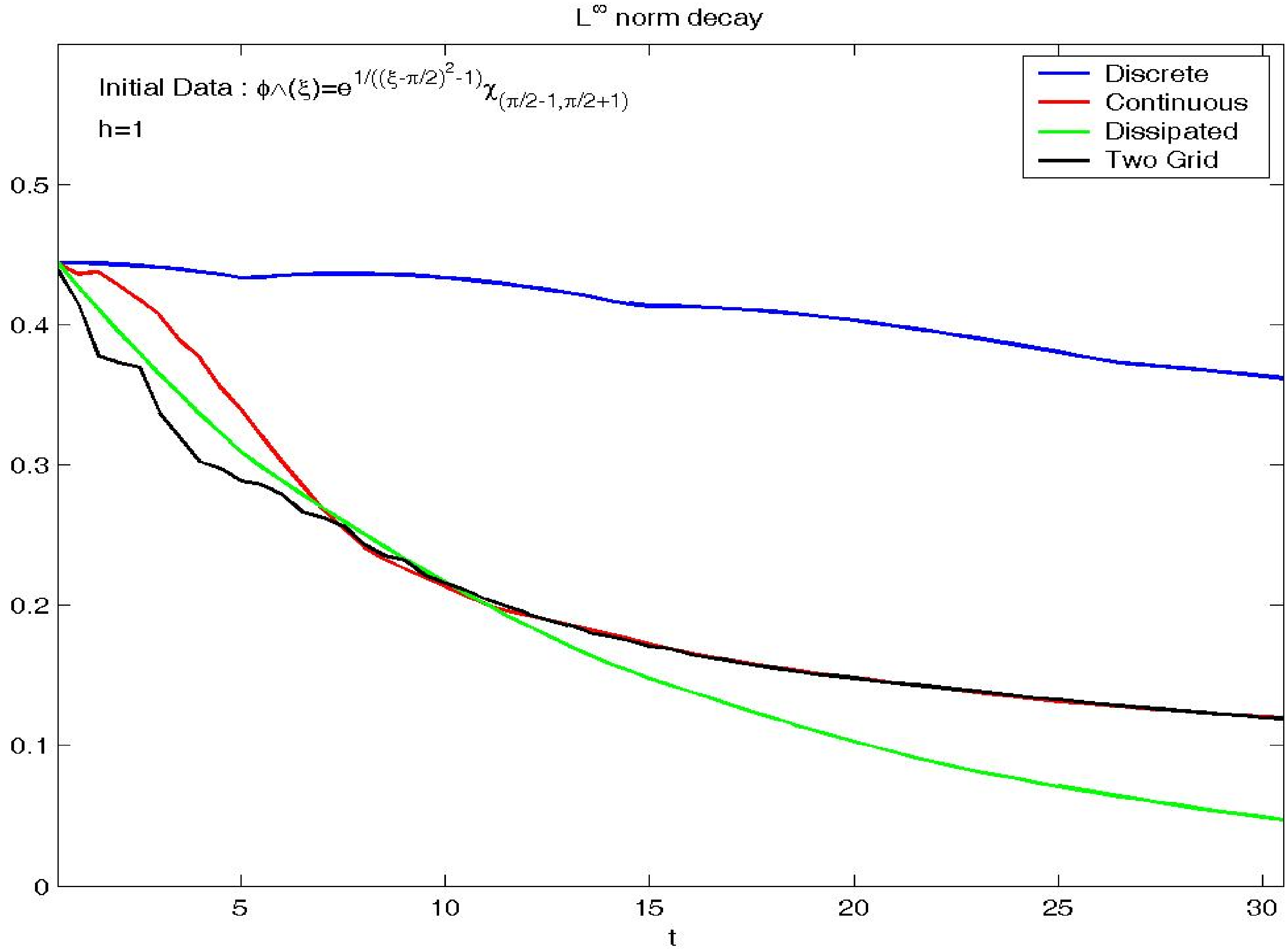
for all $\varphi^h \in l_h^q(\mathbf{Z})$ *and all* $h < 1$*.*

For $q = 2$*,* $s = \frac{1}{2}\left(\frac{1}{\alpha} - 1\right)$*. Adding numerical viscosity at a suitable scale we can reach the* H^s*-regularization for all* $s < 1/2$*, but not for the optimal case* $s = 1/2$*. This will be a limitation to deal with the critical nonlinearities. Indeed, when* $\alpha = 1/2$*,* $a(h) = 1$ *and the scheme is no longer an approximation of the Schrödinger equation itself.*

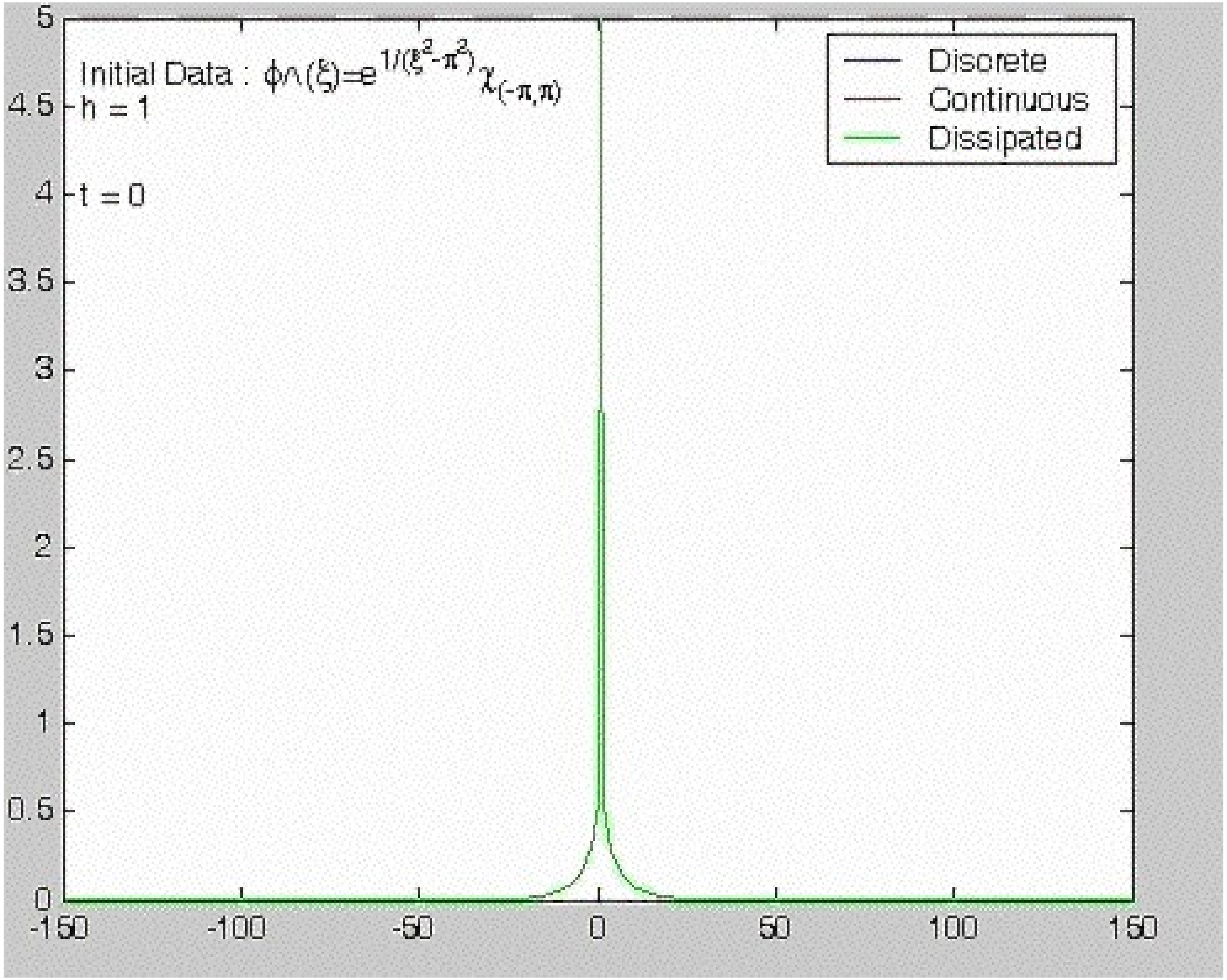
The proof:

(a) *Solutions are obtained as an iterated convolution of a discrete Schrödinger Kernel and a parabolic one. The heat kernel kills the high frequencies, while for the low ones the discrete Schrödinger kernel behaves very much the same as the continuous one.*

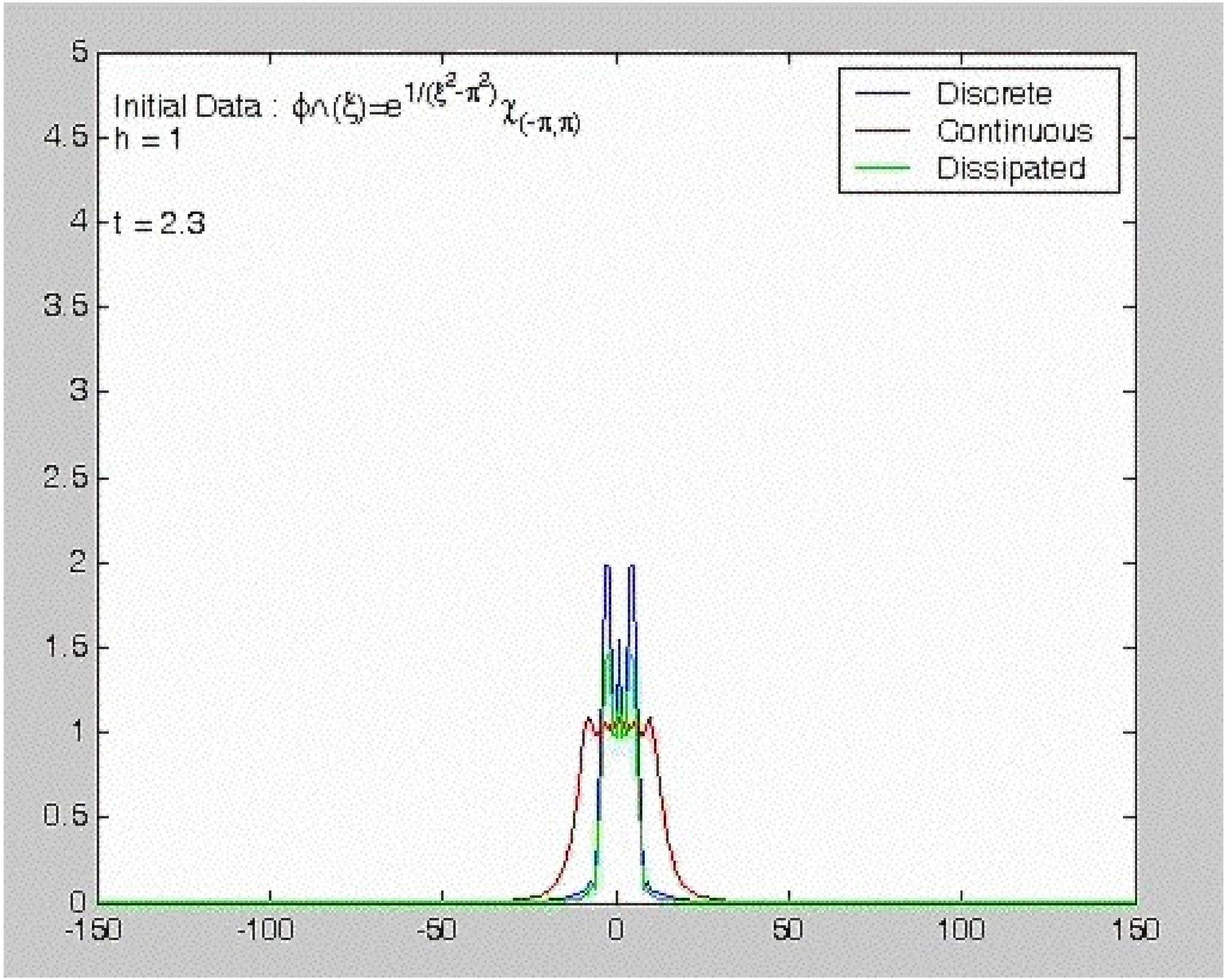
(b) *At a technical level, the proof combines the methods of Harmonic Analysis for continuous dispersive and sharp estimates of Bessel functions arising in the explicit form of the discrete heat kernel (Kenig-Ponce-Vega, Barceló-Córdoba,...).*

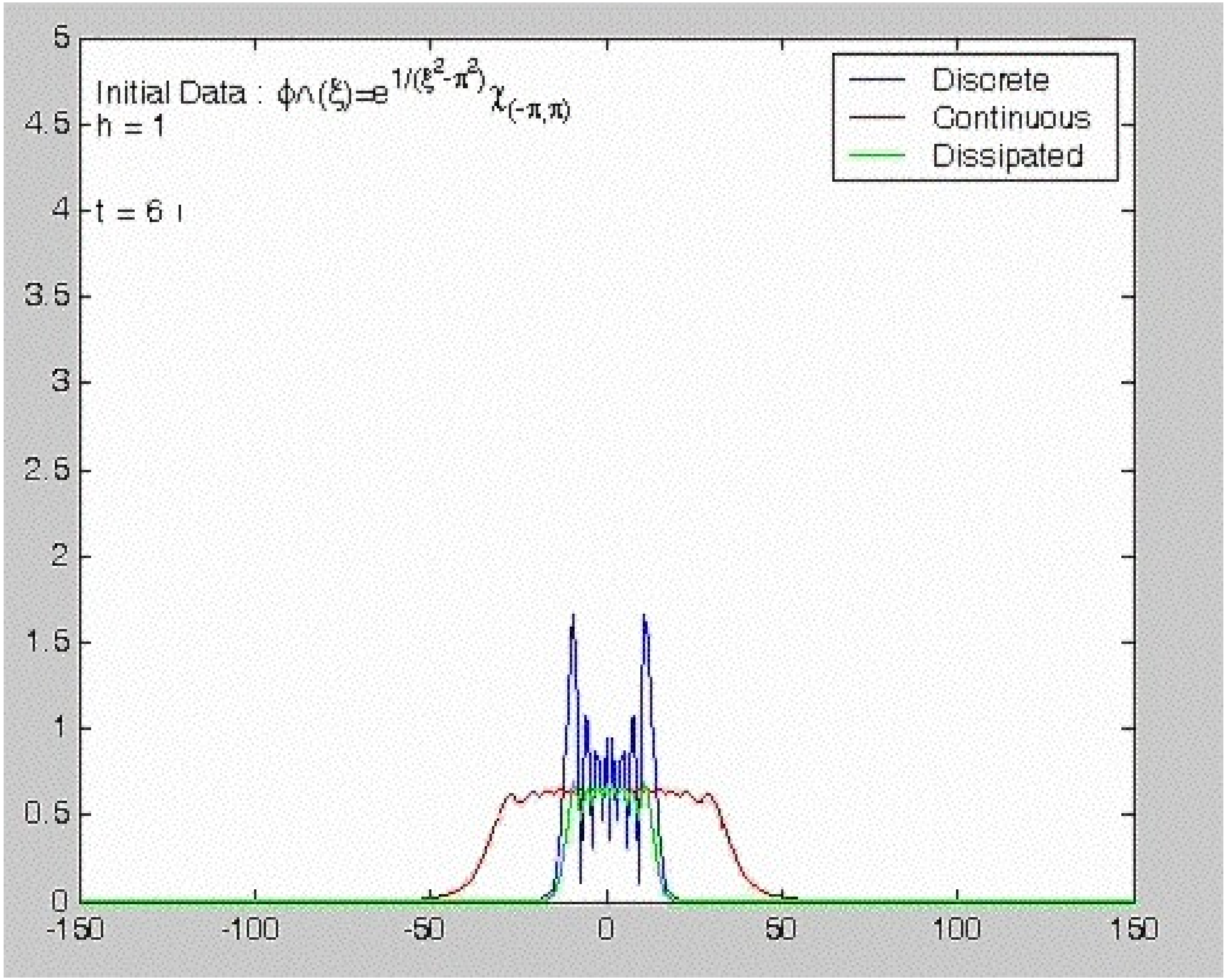


L$^\infty$ norm decay
Initial Data : $\phi\wedge(\xi)=e^{1/((\xi-\pi/2)^2-1)}\chi_{(\pi/2-1,\pi/2+1)}$
h=1
Discrete
Continuous
Dissipated
Two Grid
0.5
0.4
0.3
0.2
0.1
0
5
10
15
20
25
30
t

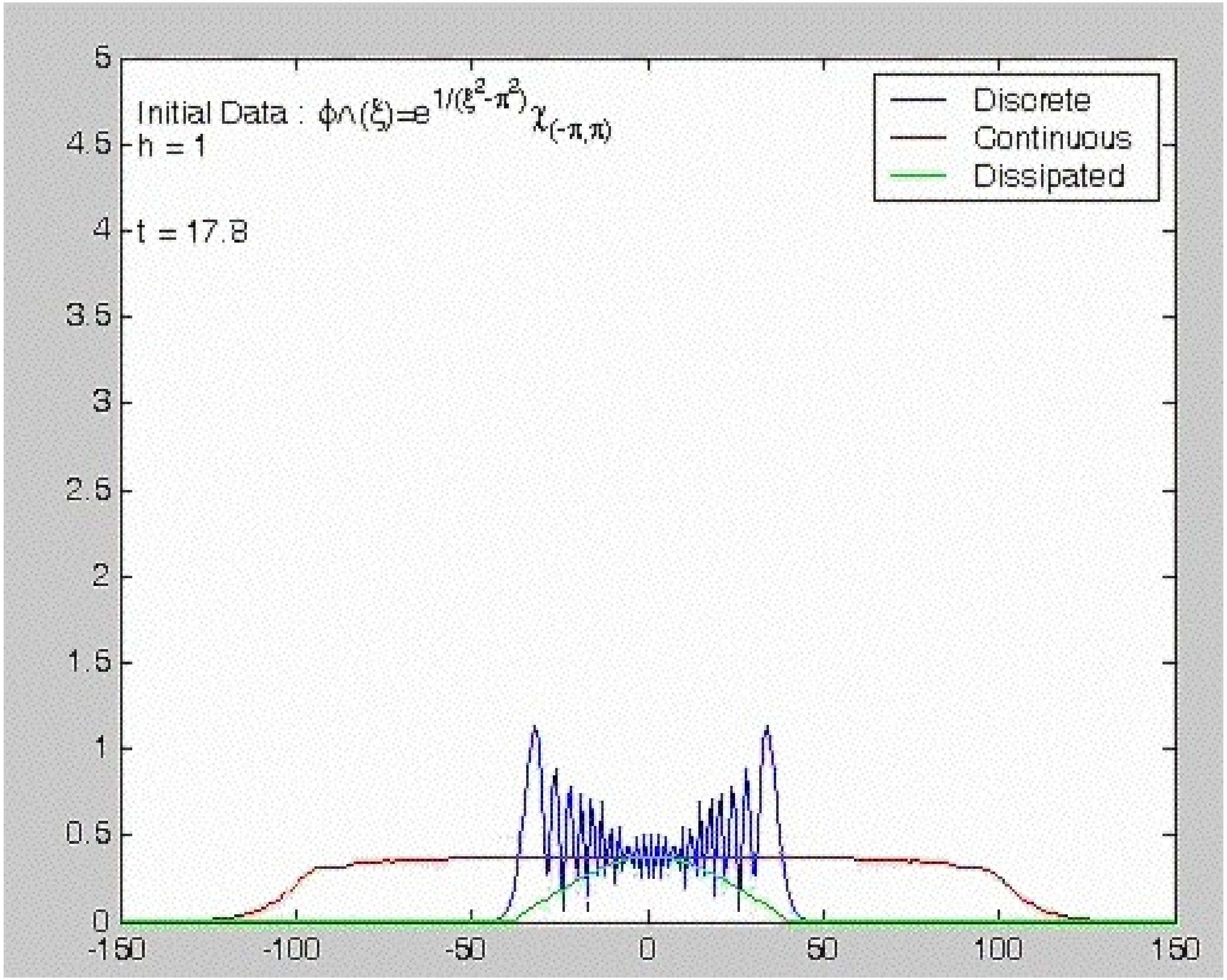


Initial Data : φ∧(ξ)=e^{1/(ξ²-π²)} χ_{(-π,π)}
h = 1
t = 0
Discrete
Continuous
Dissipated
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-150
-100
-50
0
50
100
150


Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 2.3
Discrete
Continuous
Dissipated
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-150
-100
-50
0
50
100
150



Initial Data : φ^(ξ)=e^{1/(ξ²-π²)} χ(-π,π)
h = 1
t = 6
Discrete
Continuous
Dissipated


Initial Data : φ^(ξ)=e^{1/(ξ²-π²)} χ_(-π,π)
h = 1
t = 17.8
Discrete
Continuous
Dissipated
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-150
-100
-50
0
50
100
150

NUMERICAL APPROXIMATION OF THE NLSE

Consider now:

$$\begin{cases} iu_t + u_{xx} &= |u|^p u \quad x \in \mathbf{R}, t > 0, \\ u(0,x) &= \varphi(x) \quad x \in \mathbf{R}, \end{cases} \tag{9}$$

which can also be rewritten by means of the variation of constants formula:

$$u(t) = S(t)\varphi - i \int_0^t S(t-s)|u(s)|^p u(s) ds, \tag{10}$$

where $S(t) = e^{it\Delta}$ *is the Schrödinger operator.*

Let us recall the following classical result:

Theorem 5 *(Global existence in* L^2*, Tsutsumi, 1987). For* $0 \leq p < 4$ *and* $\varphi \in L^2(\mathbf{R})$*, there exists a unique solution* u *in* $C(\mathbf{R}, L^2(\mathbf{R})) \cap L^q_{loc}(L^{p+2})$ *with* $q = 4(p+1)/p$ *that satisfies the* L^2*-norm conservation and depends continuously on the initial condition in* L^2*.*

Consider now the semi-discretization:

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = ia(h)\Delta_h u^h + |u^h|^p u^h, & t > 0 \\ u^h(0) = \varphi^h \end{cases} \tag{11}$$

with $0 < p < 4$ *and*

$$a(h) = h^{2-\frac{1}{\alpha(h)}}$$

such that

$$\alpha(h) \downarrow 1/2, \quad a(h) \to 0$$

as $h \downarrow 0$.

Then, as a consequence of the uniform (with respect to h) dispersivity properties of the linear viscous scheme:

- *The viscous semi-discrete nonlinear Schrödinger equation is globally in time well-posed;*
- *The solutions of the semi-discrete system converge to those of the continuous Schrödinger equation as $h \to 0$.*

BUT THE VISCOUS SCHEME FAILS TO BE CONSERVATIVE.

ARE THERE CONSERVATIVE REMEDIES?

A TWO-GRID ALGORITHM

Inspired on the method introduced by R. Glowinski (J. Compt. Phys., 1992) for the numerical approximation of controls for wave equations.

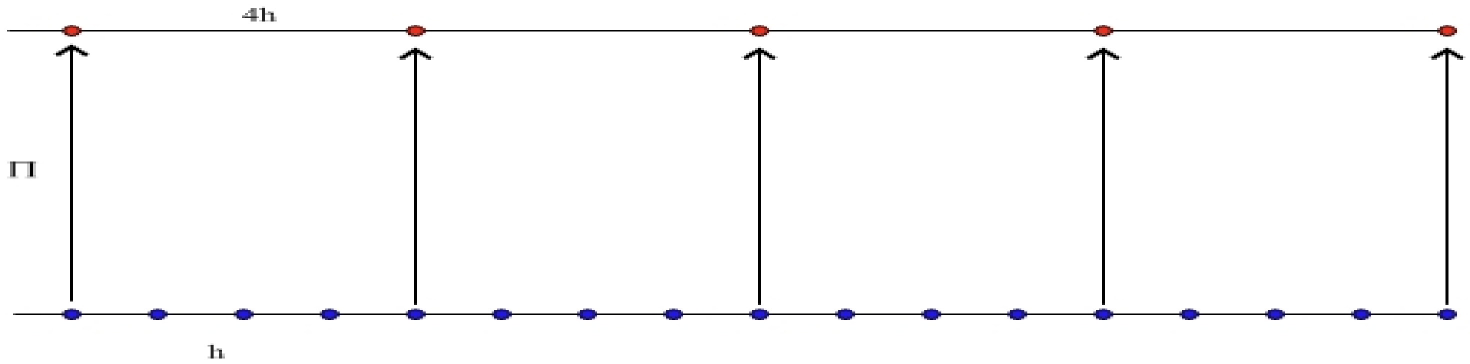
The idea: To work on the grid of mesh-size h with slowly oscillating data interpolated from a coarser grip of size $4h$. The ratio $1/2$ of meshes does not suffice for the present problem!

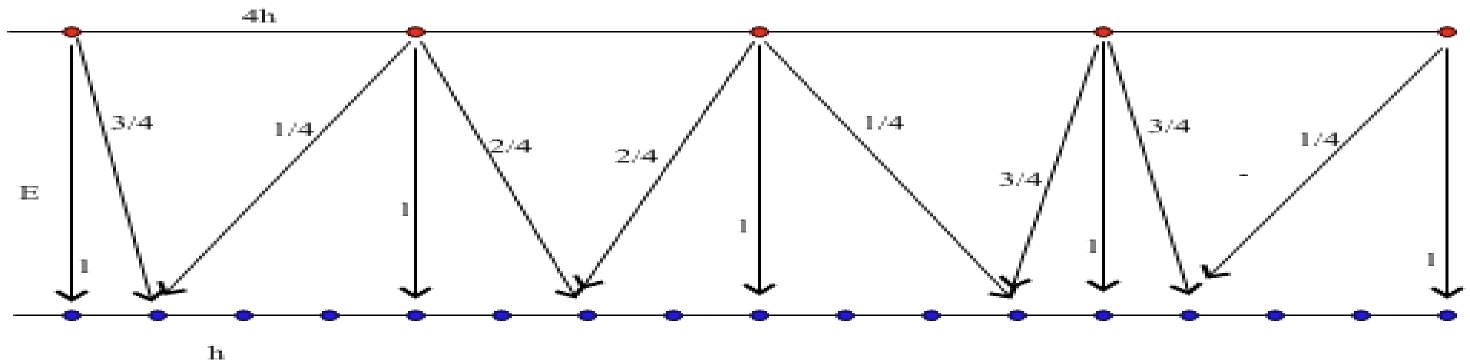
The space of discrete functions on the coarse mesh $4h\mathbf{Z}$:

$$\mathbb{C}_4^{h\mathbf{Z}} = \{\psi \in \mathbb{C}^{h\mathbf{Z}} : \mathrm{supp}\,\psi \subset 4h\mathbf{Z}\},$$

and the extension operator E:

$$(E\psi)((4j+r)h) = \frac{4-r}{4}\psi(4jh) + \frac{r}{4}\psi((4j+4)h),\ \forall j \in \mathbf{Z}, r = \overline{0,3}, \psi \in \mathbb{C}_4^{h\mathbf{Z}}.$$


4h
Π
h


4h
E
3/4
1/4
2/4
2/4
1/4
3/4
3/4
1/4
1
1
1
1
1
1
h

Let V_4^h be the space of slowly oscillating sequences (SOS) on the fine grid

$$V_4^h = \{E\psi : \psi \in C_4^{h\mathbf{Z}}\},$$

and the projection operator $\Pi : \mathbb{C}^{h\mathbf{Z}} \to \mathbb{C}_4^{h\mathbf{Z}}$:

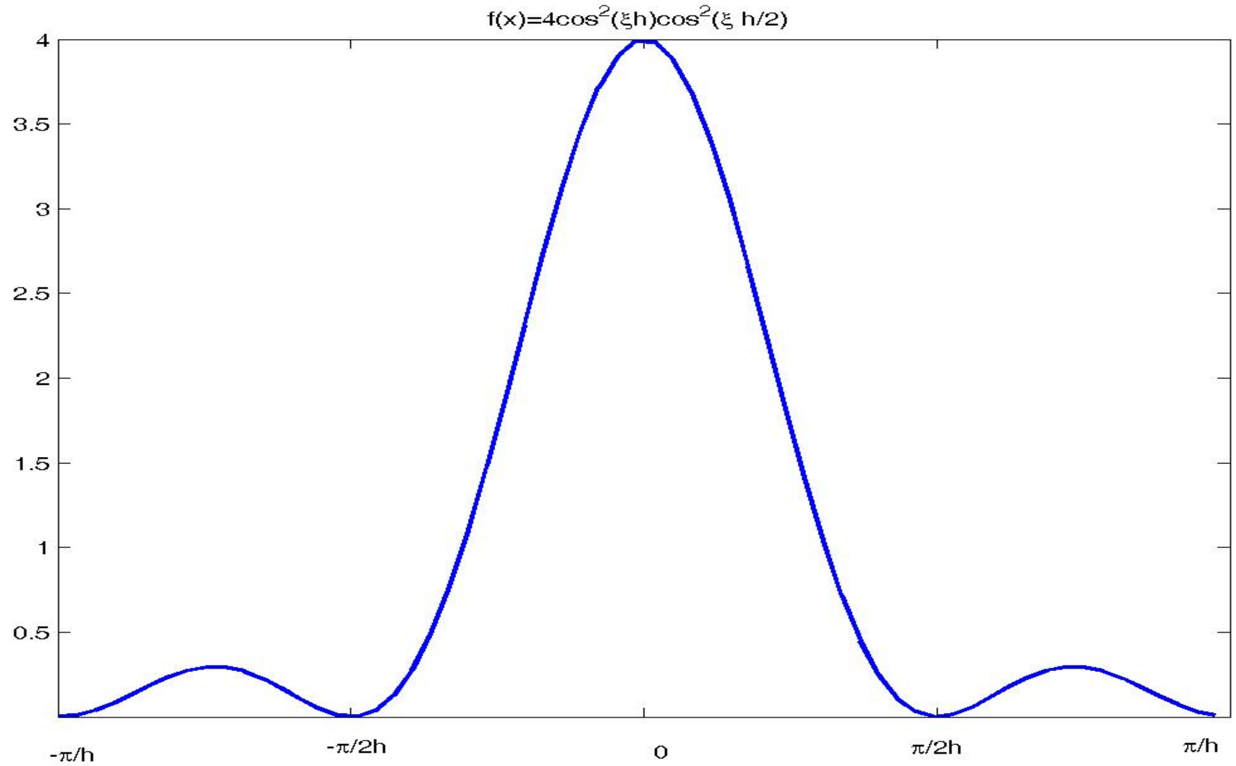
$$(\Pi\phi)((4j+r)h) = \phi((4j+r)h)\delta_{4r}, \forall j \in \mathbf{Z}, r = \overline{0,3}, \phi \in \mathbb{C}^{h\mathbf{Z}}.$$

We now define the smoothing operator

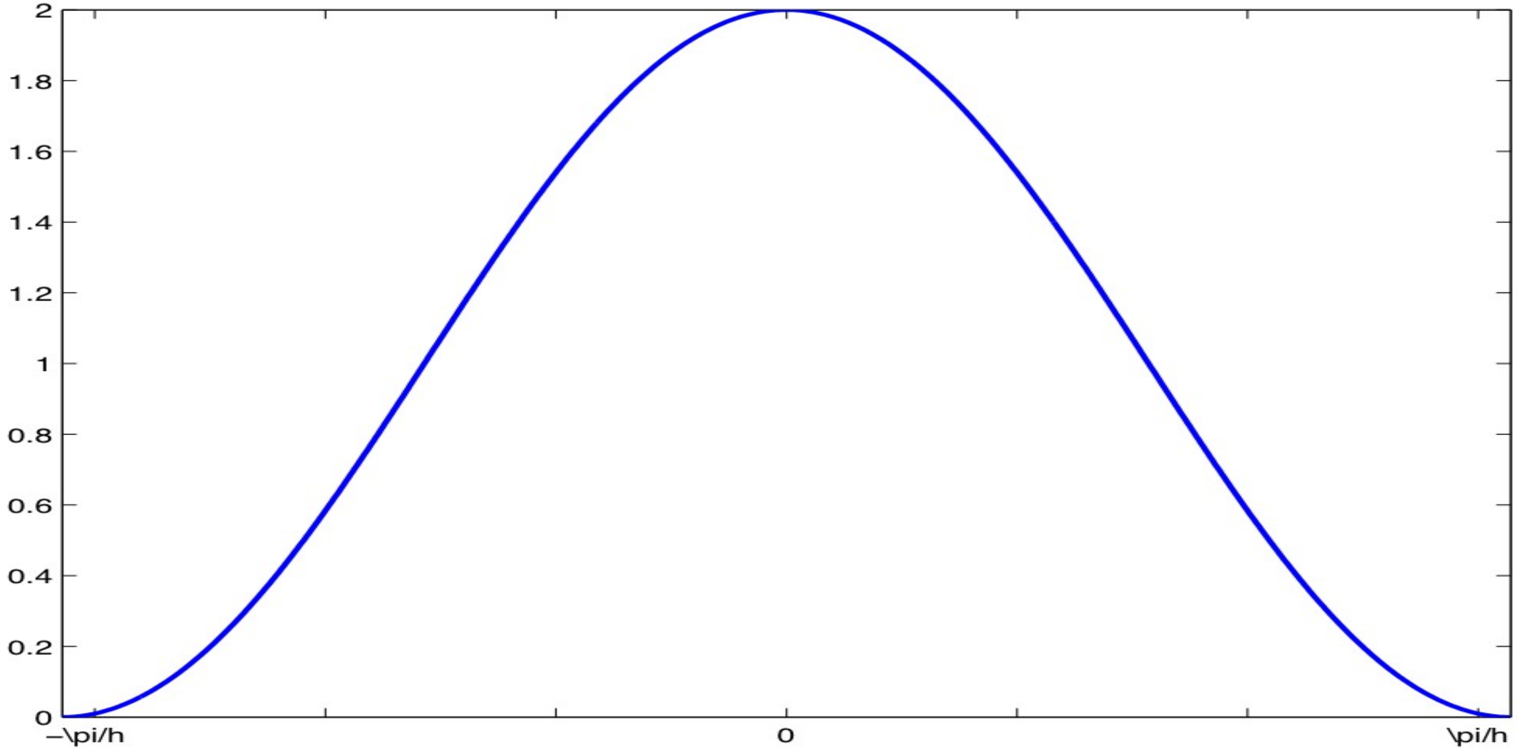
$$\tilde{\Pi} = E\Pi : \mathbb{C}^{h\mathbf{Z}} \to V_4^h,$$

which acts as a a filtering, associating to each sequence on the fine grid a slowly oscillating sequence. The discrete Fourier transform of a slowly oscillating sequence SOS is as follows:

$$\widehat{\tilde{\Pi}\phi}(\xi) = 4\cos^2(\xi h)\cos^2(\xi h/2)\widehat{\Pi\phi}(\xi).$$



Amplification factor for the grid method with ratio 1/2.



Amplification factor for the two-grid method with ratio $1/4$.

Insufficient to filter the pathological frequencies $\pm\pi/2h$.

Dispersion properties: The semi-discrete Schrödinger semigroup when acting on SOS has the same properties as the continuous Schrödinger equation:

Theorem 6 *i) For* $p \geq 2$,

$$\left| e^{it\Delta_h} \widetilde{\Pi}\varphi \right|_{l^p(h\mathbf{Z})} \lesssim |t|^{-1/2(1/p'-1/p)} \left| \widetilde{\Pi}\varphi \right|_{l^{p'}(h\mathbf{Z})}.$$

ii) Furthermore, for every admissible pair (q, r),

$$\left| e^{it\Delta_h} \widetilde{\Pi}\varphi \right|_{L^q(\mathbb{R}, l^r(h\mathbf{Z}))} \lesssim \left| \widetilde{\Pi}\varphi \right|_{l^2(h\mathbf{Z})}.$$

SOS sequences vanish at $\pm\pi/2$. *This implies the gain of integrability.*

Sketch of the Proof. By scaling, we can assume that $h = 1$. We write $T(t)$ as a convolution operator $T(t)\psi = K^t * \psi$ where

$$\widehat{K^t}(\xi) = 4e^{-4it\sin^2\xi/2}\cos^2\xi\cos^2(\xi/2).$$

We need

$$\left|K^t\right|_{l^\infty(\mathbf{Z})} \lesssim 1/\sqrt{t}.$$

The fact that $(4\sin^2(\xi/2))'' = 2\cos(\xi)$ allows applying the sharp results by Kenig-Ponce-Vega and Keel-Tao to derive the desired decay.

Concerning the local smoothing properties we can prove that

Theorem 7 *Let $r \in (1, 2]$. Then*

$$\sup_{j\in\mathbf{Z}} \int_{-\infty}^{\infty} \left|(D^{1-1/r} e^{it\Delta_h} \widetilde{\Pi} f)_j\right|^2 dt \lesssim \left|\widetilde{\Pi} f\right|^2_{l^r(h\mathbf{Z})} \tag{12}$$

for all $f \in l^r(h\mathbf{Z})$, uniformly in $h > 0$.

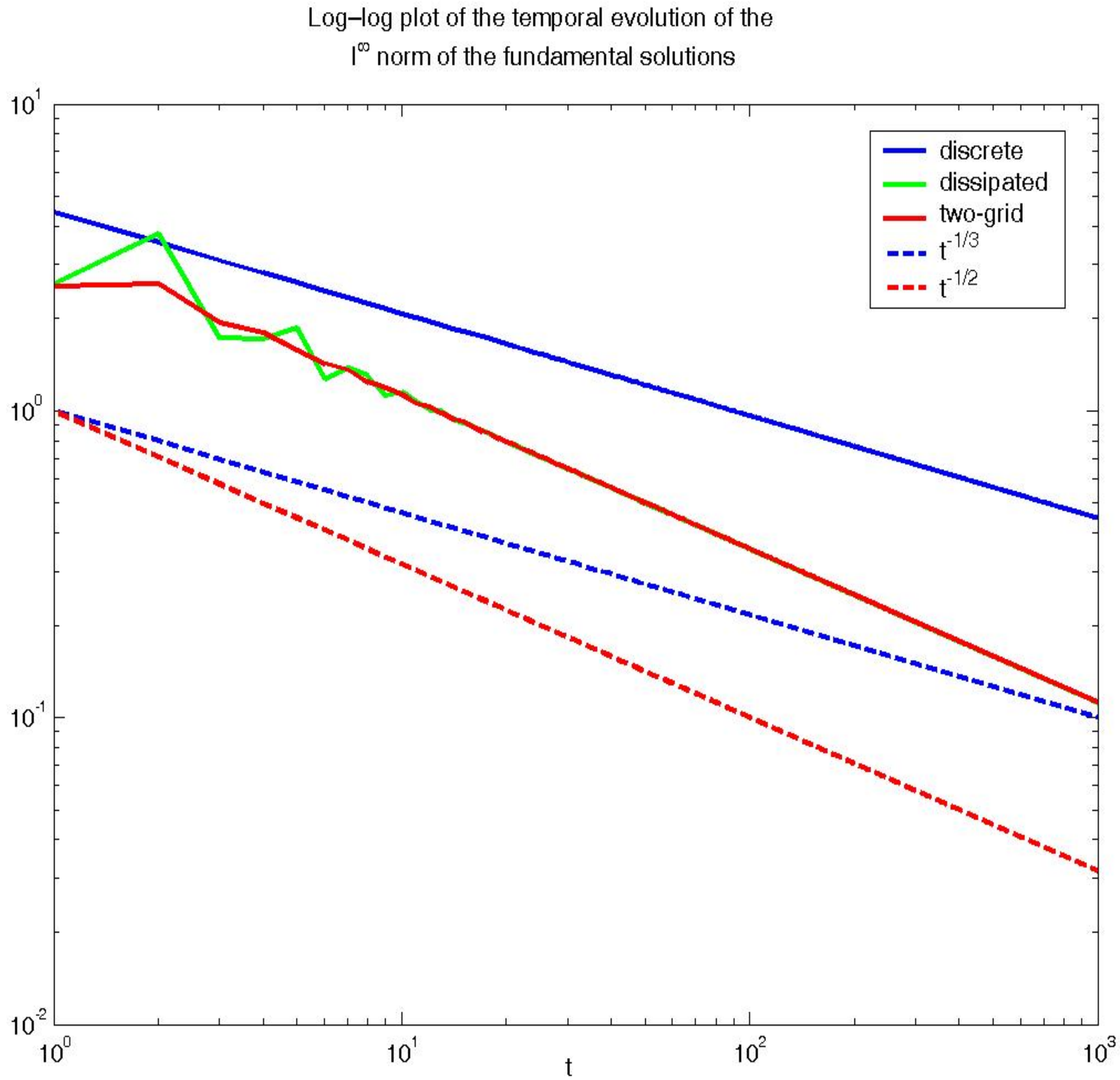
SOS vanish at the spectral points $\xi = \pm\pi/h$. This implies gain of local regularity.

Sketch of the Proof. *Applying results by Kenig-Ponce-Vega we have to* T_1 *we get*

$$\sup_{x\in\mathbb{R}} \int_{-\infty}^{\infty} |(T_1(t)\varphi)(x)|^2\, dt \lesssim \int_{-\pi}^{\pi} \frac{|\hat{f}(\xi)|^2 \cos^4\xi \cos^4(\xi/2)}{|\sin\xi|} d\xi.$$

Then, using the fact that $\cos^4\xi \cos^4(\xi/2)$ *vanishes at* $\xi = \pm\pi$, *we can compensate the singularity of* $\sin(\xi)$ *in the denominator and guarantee that*

$$\sup_{x\in\mathbb{R}} \int_{-\infty}^{\infty} |(T_1(t)\varphi)(x)|^2\, dt \lesssim \int_{-\pi}^{\pi} \frac{|\hat{f}(\xi)|^2}{|\xi|} d\xi \lesssim \left| D^{-1/2} f \right|_{L^2(\mathbb{R})}^2.$$


Log–log plot of the temporal evolution of the
l^∞ norm of the fundamental solutions
discrete
dissipated
two-grid
$t^{-1/3}$
$t^{-1/2}$
10^1
10^0
10^{-1}
10^{-2}
10^0
10^1
10^2
10^3
t

In view of the uniform dispersion properties of the two-grip approximation scheme, the method guarantees convergence for nonlinear problems too.

The two-grid algorithm allows building conservative convergent schemes for nonlinear Schrödinger equations in the sharp class of nonlinearities in which the continuous PDE is well-posed.

Things improve further when we also discretize in time.

Time discretization $\sim$ *time upwind* $\sim$ *time viscosity* $\sim$ *space-like viscosity.*

CONCLUSIONS:

- MANY SYSTEMS OF PDE DEVELOP FINE QUALITATIVE PROPERTIES THAT STANDARD NUMERICAL SCHEMES DO NOT NECESSARILY CAPTURE.

- FURTHER AND FINE ANALYSIS IS NEEDED TO INVESTIGATE WHETHER NUMERICAL SCHEMES BEHAVE IN A STABLE WAY WITH RESPECT TO THESE PROPERTIES, AND TO DEVELOP REMEDIES, WHEN NEEDED.

- FOURIER FILTERING (AND SOME OTHER VARIANTS LIKE NUMERICAL VISCOSITY, TWO-GRIDS...) ALLOW BUILDING EFFICIENT NUMERICAL SCHEMES.

- *THESE NEW SCHEMES ALLOW CAPTURING THE RIGHT DISPERSION PROPERTIES OF THE CONTINUOUS MODELS AND CONSEQUENTLY PROVIDE CONVERGENT APPROXIMATIONS FOR NONLINEAR EQUATIONS TOO.*

- *IN PRACTICE THE TWO-GRID METHOD IS EASIER TO APPLY IN A SYSTEMATIC WAY. IT MAY ALSO BE EASIER TO ADAPT TO GENERAL NON-REGULAR MESHES.*

- *THE METHODS DEVELOPED IN THIS CONTEXT ARE STRONGLY INSPIRED ON OUR PREVIOUS WORK ON THE NUMERICAL APPROXIMATION OF CONTROLS FOR WAVE EQUATIONS.*

- *MUCH REMAINS TO BE DONE IN ORDER TO DEVELOP A COMPLETE THEORY (MULTIDIMENSIONAL PROBLEMS,*

BOUNDARY-VALUE PROBLEMS, NONREGULAR MESHES, OTHER PDE'S,...)

- A COMPLETE THEORY SHOULD COMBINE FINE HARMONIC ANALYSIS, MULTIRESOLUTION ANALYSIS, NUMERICAL ANALYSIS AND PDE THEORY.

- THE SAME IDEAS SHOULD BE USEFUL TO DEAL WITH OTHER ISSUES SUCH AS TRANSPARENT BOUNDARY CONDITIONS, SCATTERING PROBLEMS, ...

Gracias !

Thank you!