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Dispersive equations and numerical approximation

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THE GENERAL PROBLEM:

TO BUILD CONVERGENT NUMERICAL SCHEMES FOR NON-LINEAR PARTIAL DIFFERENTIAL EQUATIONS (PDE).

Example: SCHRÖDINGER EQUATION.

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

Goal: To cover the classes of NONLINEAR Schrödinger equations that can be solved nowadays with fine tools from PDE theory and Harmonic analysis.

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?

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

UNDERLYING MAJOR PROBLEM:

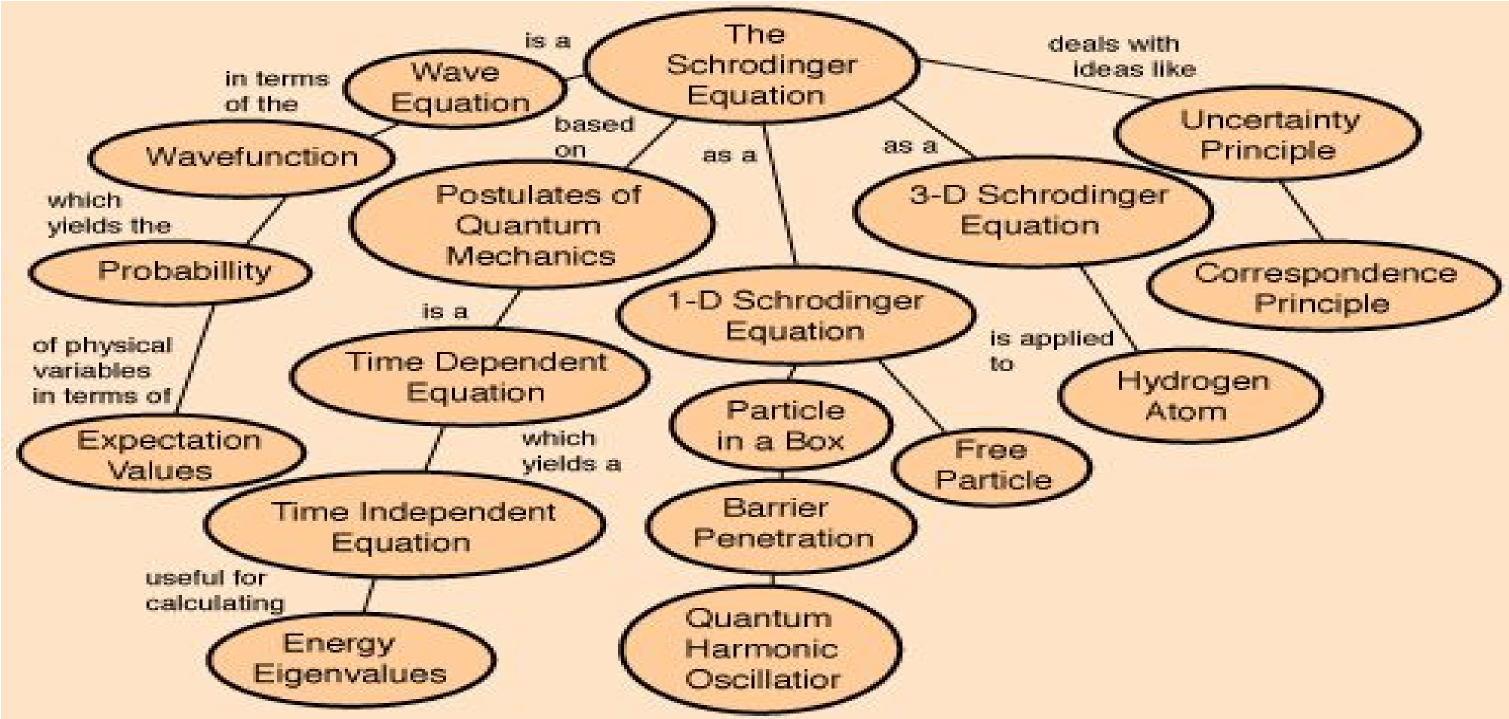
Reproduce in the computer the dynamics in Continuum and Quantum Mechanics, avoiding spurious numerical solutions.

The issue can only be understood by adapting at the discrete numerical level the techniques developed in the continuous context.

WARNING!

NUMERICS = CONTINUUM + (POSSIBLY) SPURIOUS

MOTIVATION/APPLICATIONS

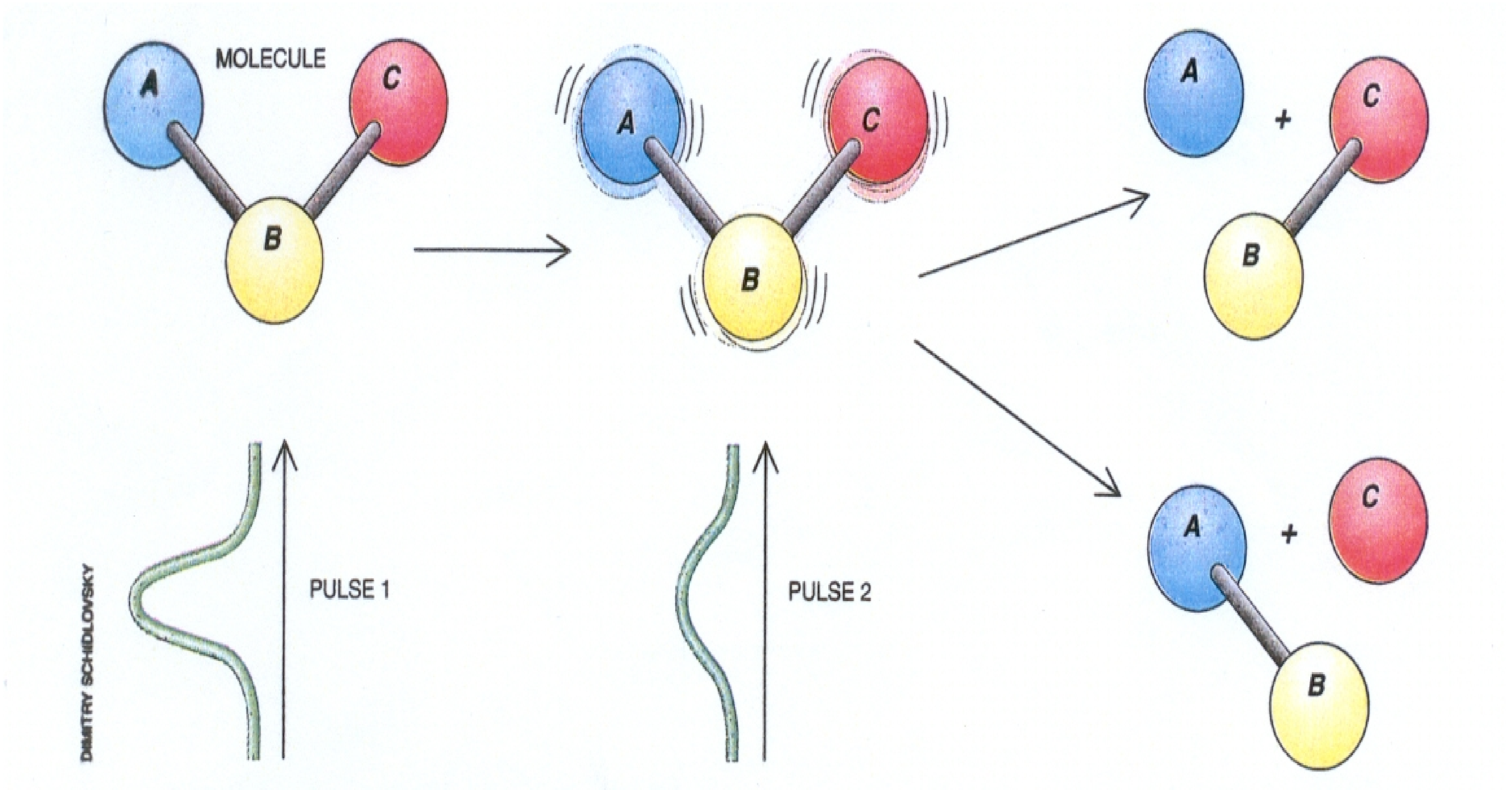


http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/schrcn.html#c1

- Quantum control and Computing.

  Laser control in Quantum mechanical and molecular systems to design coherent vibrational states.

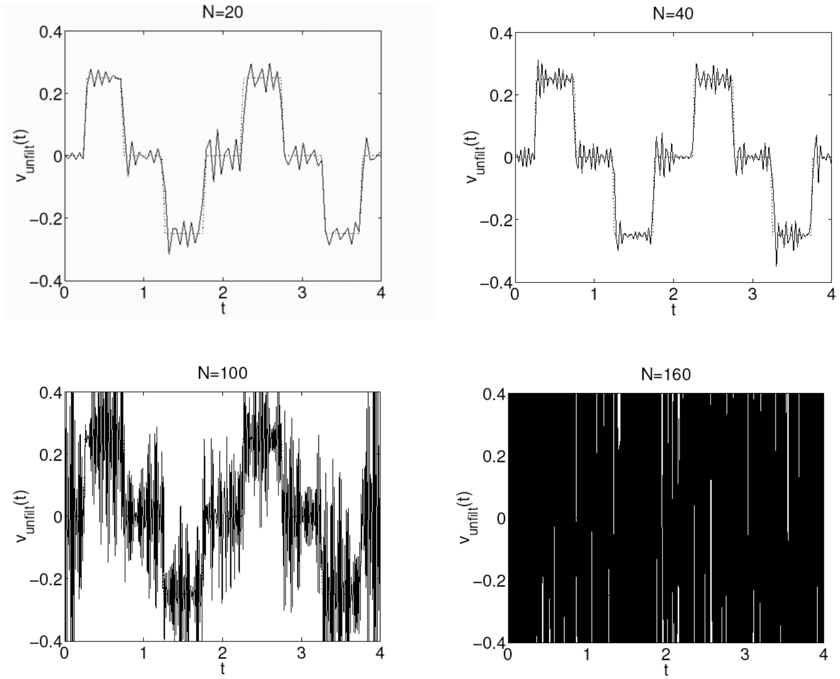
  In this case the fundamental equation is the Schrödinger one. The Schrödinger equation may be viewed as a wave equation with inifnite speed of propagation.



P. Brumer and M. Shapiro, Laser Control of Chemical reactions, Scientific American, March, 1995, pp.34-39.

Strongly inspired in our previous work on the CONTROL OF WAVE PHENOMENA

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



PRELIMINARIES I: THE ABSTRACT FORMULATION OF A PDE

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

A an unbounded operator in a Hilbert (or Banach) space H, with domain $D(A) \subset H$.

The solution is given by

$$u(t) = e^{At}u_0.$$

Semigroup theory provides conditions under which e^{At} is well defined. Roughly A needs to be *maximal* ($A + I$ is invertible) and *dissipative* ($A \leq 0$).

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

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

$$f : H \longrightarrow H \text{ is locally Lipschitz},$$

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 $p > 1$.

In order for this procedure to be applied one needs to discover other properties of the underlying linear equation (smoothing, dispersion). Whenever e^{At} has the property that

$$e^{At}u_0 \in X,$$

then, it is natural to look for solutions of the nonlinear problem in

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

One then needs to investigate whether $f : C([0,T];H) \cap X \to C([0,T];H) \cap X$ is locally Lipschitz. This requires extra work: We need to test the behavior of f in the space X. But the the class of functions to be tested is restricted to those belonging to 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.

PRELIMINARIES II: NUMERICAL ANALYSIS

Replace the PDE $u_t(t) + Au(t) = 0$ by a discrete scheme that a computer might solve.

$A \sim A_h$, A_h being a discrete operator.

$A_h \to A$, as $h \to 0$.

The continuous derivatives are replaced by discrete ones according to Taylor's expansions.

The new problem becomes:

$$u_t(t) = A_h u(t), \quad t \geq 0; \quad u(0) = u_0.$$

It is now typically a finite-dimensional system of ODE.

One can finally apply the standard theory of numerical analysis for ODE, to replace it by a purely discrete scheme. For instance:

$$u^{k+1} = u^k + (\Delta t) A_h u^k,$$

$k \geq 1$, which arises naturally when replacing $u_t = \frac{du}{dt}$ by $\frac{u^{k+1} - u^k}{\Delta t}$.

THE MAIN QUESTION:

DOES THE NUMERICAL SCHEME CONVERGE?

$$\max_{0 \leq t \leq T} ||u(t) - u_h(t)||_H \to 0, \quad as \quad h \to 0.??????$$

According to P. Lax's Theorem,

$$\text{CONVERGENCE} = \text{CONSISTENCY} + \text{STABILITY.}$$

Consistency: The numerical scheme is in agreement with the rules of Differential Calculus, so that the discretization approximates the differential operator involved in the PDE, and not another one!. Consistency means that the scheme is "reasonable".

Stability: The numerical scheme should be so that all trajectories remain uniformly bounded.

$$\sup_{h>0} \max_{0 \leq t \leq T} ||u_h(t)||_H < \infty.$$

It holds immediately if $A_h \leq 0$, i. e. if the numerical scheme is dissipative as well.

The same analysis suffices to deal with nonlinear equations provided the non-linear term $f : H \rightarrow H$ is locally Lipschitz. It suffices to replace

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

by

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

and to combine:

- the convergence result for the linear problem;
- a fixed point argument;
- the variations of constants formula.

BUT IF WORKING IN $C([0,T];: H) \cap X$ WAS NEEDED FOR THE CONTINUOUS PROBLEM, IT IS HOPELESS TO PROVE CONVERGENCE OF THE NUMERICAL SCHEME IF IT DOES NOT HAVE AND APPROPRIATE BEHAVIOR IN X (OR X_h) AS WELL.

THIS OFTEN FAILS!

The Linear Schrödinger Equation (LSE):

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

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 three-point finite-difference scheme

Consider the finite difference approximation

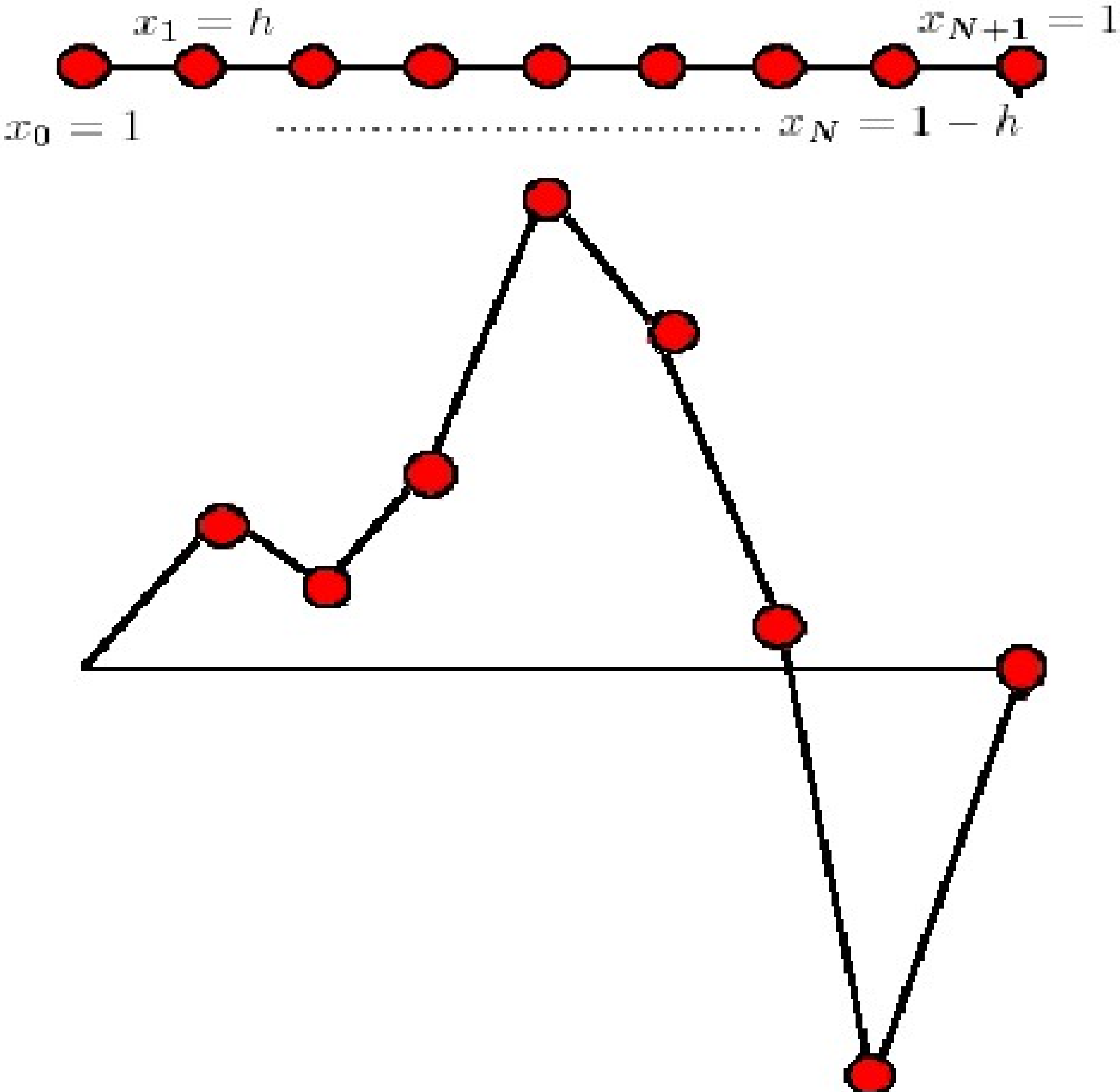
$$i\frac{du^h}{dt} + \Delta_h u^h = 0, t \neq 0, \quad u^h(0) = \varphi^h. \tag{2}$$

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 $O(h^2)$).

In fact, $||u^h(t)||_{\ell^2} = ||\varphi||_{\ell^2}$, for all $t \geq 0$.



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

The same convergence result holds for semilinear equations

$$\begin{cases} iu_t + u_{xx} &= f(u) \quad x \in \mathbf{R}, t > 0, \\ u(0,x) &= \varphi \quad x \in \mathbf{R}, \end{cases} \tag{3}$$

provided the nonlinearity $f : \mathbf{R} \to \mathbf{R}$ is globally Lipschitz.

The proof is completely standard and only requires the L^2-conservation property of the continous and discrete equation.

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

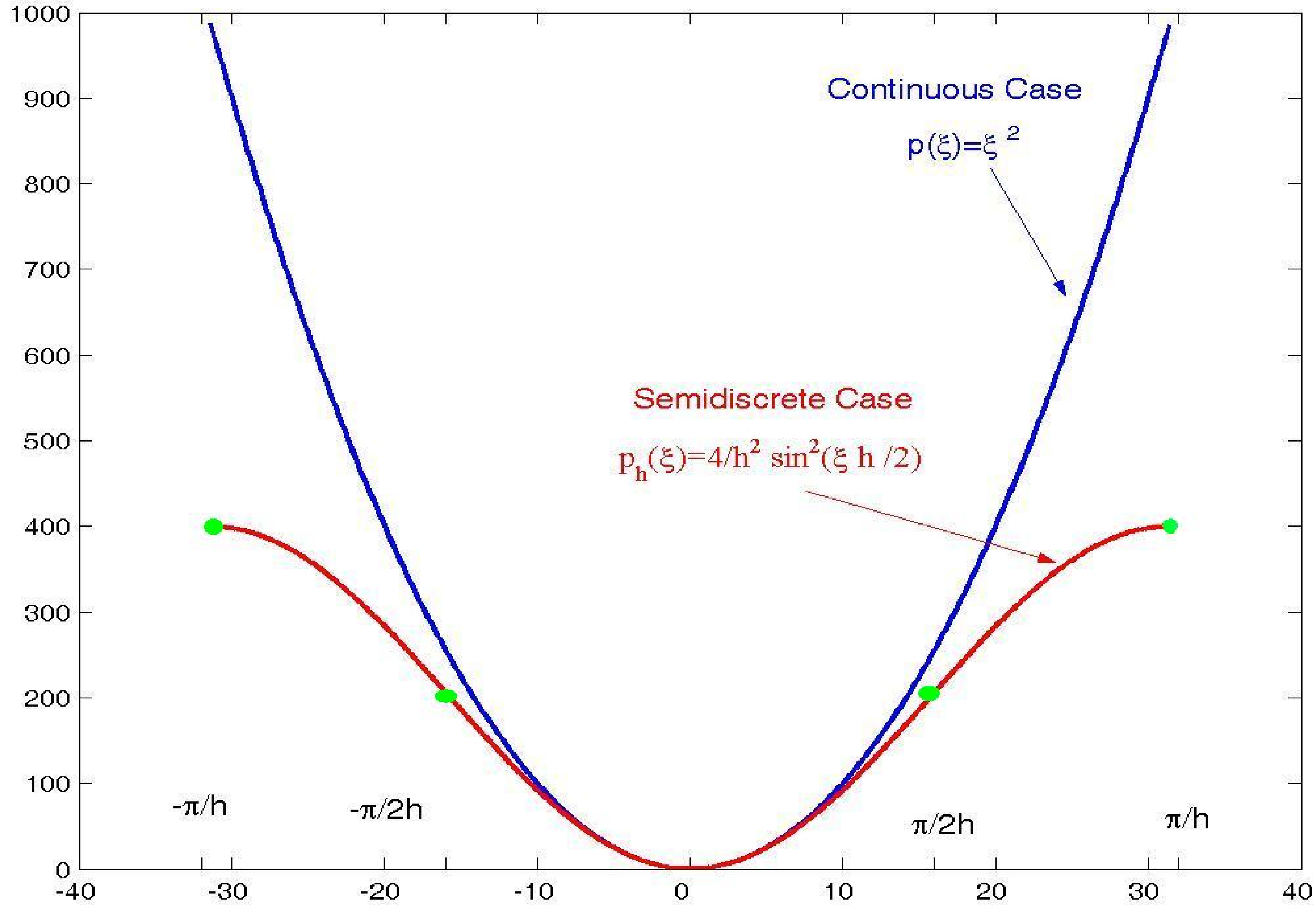
Consider the semi-discrete Fourier Transform

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

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/h^2 sin^2(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, as we shall see, this produces the lack of uniform (in h) dispersion of the numerical scheme and consequently, makes the scheme useless for nonlinear problems.

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,*

$$\sup_{h>0, \varphi^h \in l_h^{q_1}(\mathbf{Z})} \frac{|| \exp(it\Delta_h)\varphi^h ||_{l_h^{q_2}(\mathbf{Z})}}{||\varphi^h||_{l_h^{q_1}(\mathbf{Z})}} = \infty. \tag{4}$$

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

LACK OF CONVEXITY = LACK OF LAPLACIAN.

A. Stefanov & P. G. Kevrekidis, Nonlinearity 18 (2005) 18411857.

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*

$$\left| \int_a^b e^{it\phi(\xi)} d\xi \right| \leq c_k t^{-1/k} \tag{5}$$

LACK OF SLOPE= LACK OF REGULARITY GAIN.

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

$$\sup_{h>0, \varphi^h \in l_h^q(\mathbf{Z})} \frac{\left| S^h(t)\varphi^h \right|_{\hbar^s_{loc}(\mathbf{Z})}}{\left| \varphi^h \right|_{l_h^q(\mathbf{Z})}} = \infty. \tag{6}$$

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

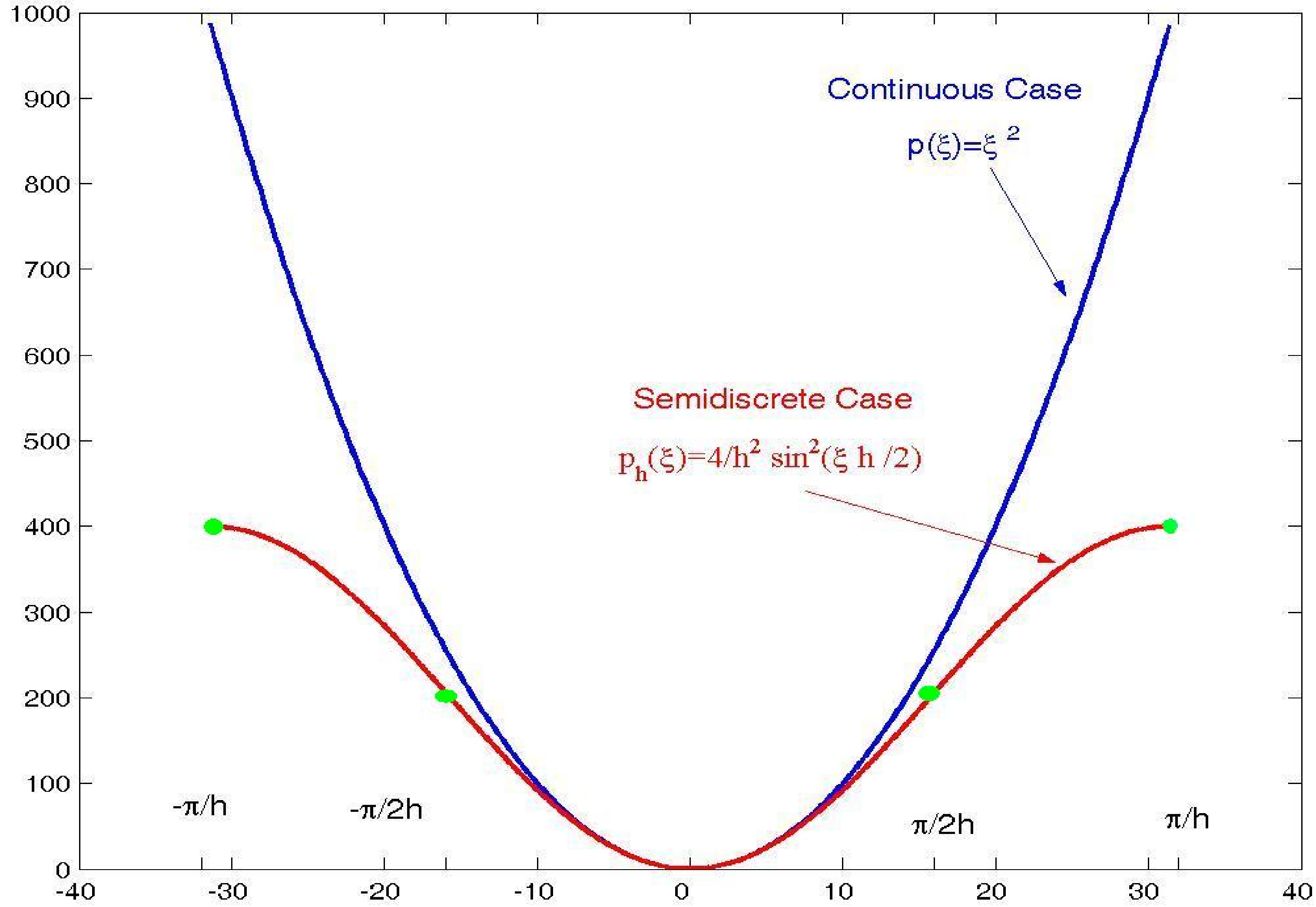
$$u_j(t) = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} e^{ijh\xi} e^{ip_h(\xi)t} \hat{\varphi}(\xi) d\xi, \quad j \in \mathbf{Z}.$$

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.



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

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h &= ia(h)\Delta_h u^h, \quad t > 0, \\ u^h(0) &= \varphi^h, \end{cases} \tag{7}$$

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* $t > 0$*:*

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

This is a 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* $u^h_t - a(h)\Delta_h u^h = 0$ *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".

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*

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

$S^h_\pm(t)$ maps continuously $l^{p'}_h(\mathbf{Z})$ to $l^p_h(\mathbf{Z})$ and there exists some positive constants $c(p)$ such that

$$||S^h_\pm(t)\varphi^h||_{l^p_h(\mathbf{Z})} \leq c(p)(|t|^{-\alpha(1-\frac{2}{p})} + |t|^{-\frac{1}{2}(1-\frac{2}{p})})||\varphi^h||_{l^{p'}_h(\mathbf{Z})} \qquad (8)$$

holds for all $|t| \neq 0$, $\varphi \in l^{p'}_h(\mathbf{Z})$ 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*

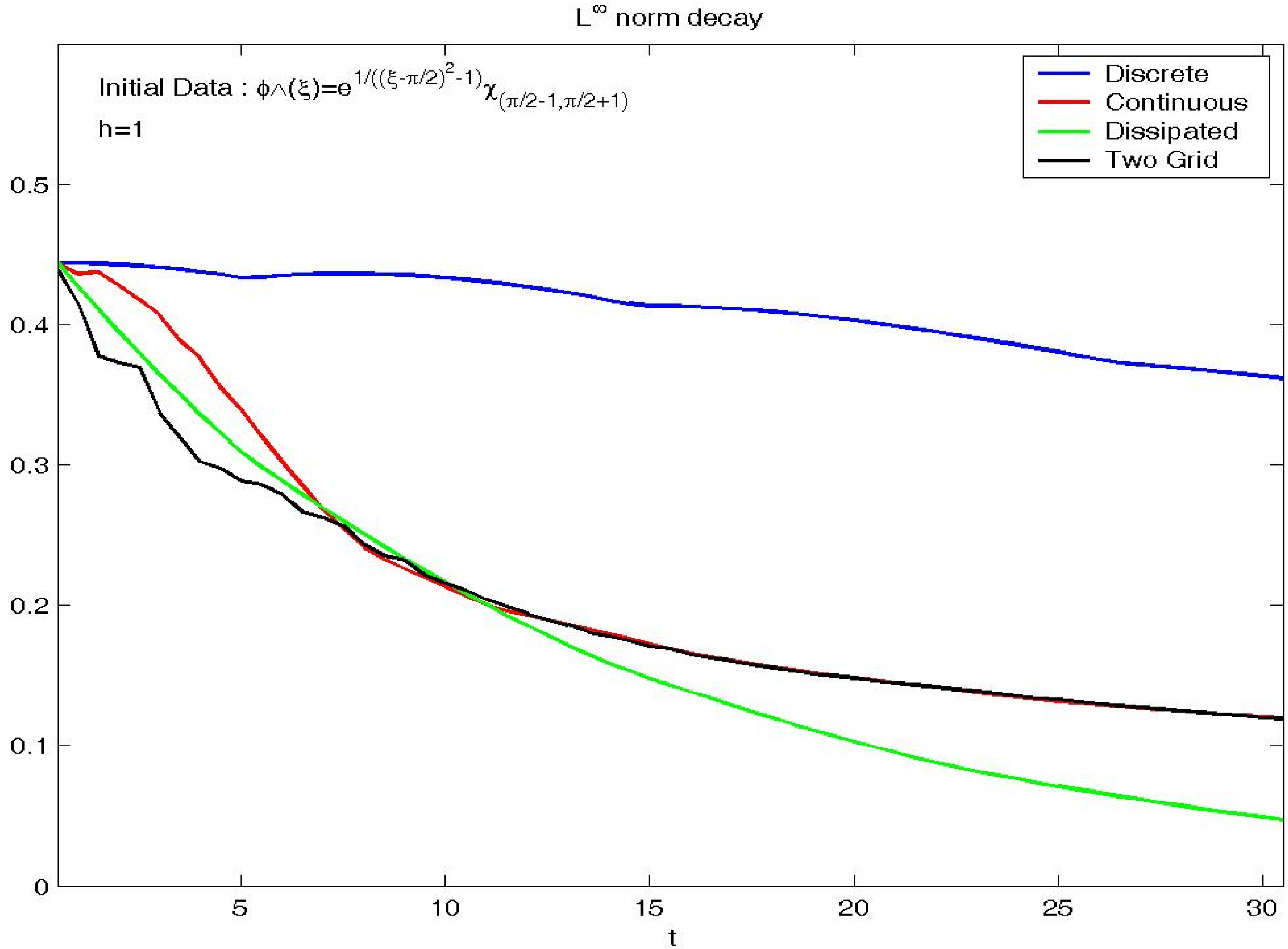
$$\left|\psi E^h u^h(t)\right|_{L^2(I;H^s(\mathbf{R}))} \leq C(I, \psi, q, s)\left|\varphi^h\right|_{l_h^q(\mathbf{Z})}. \tag{9}$$

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

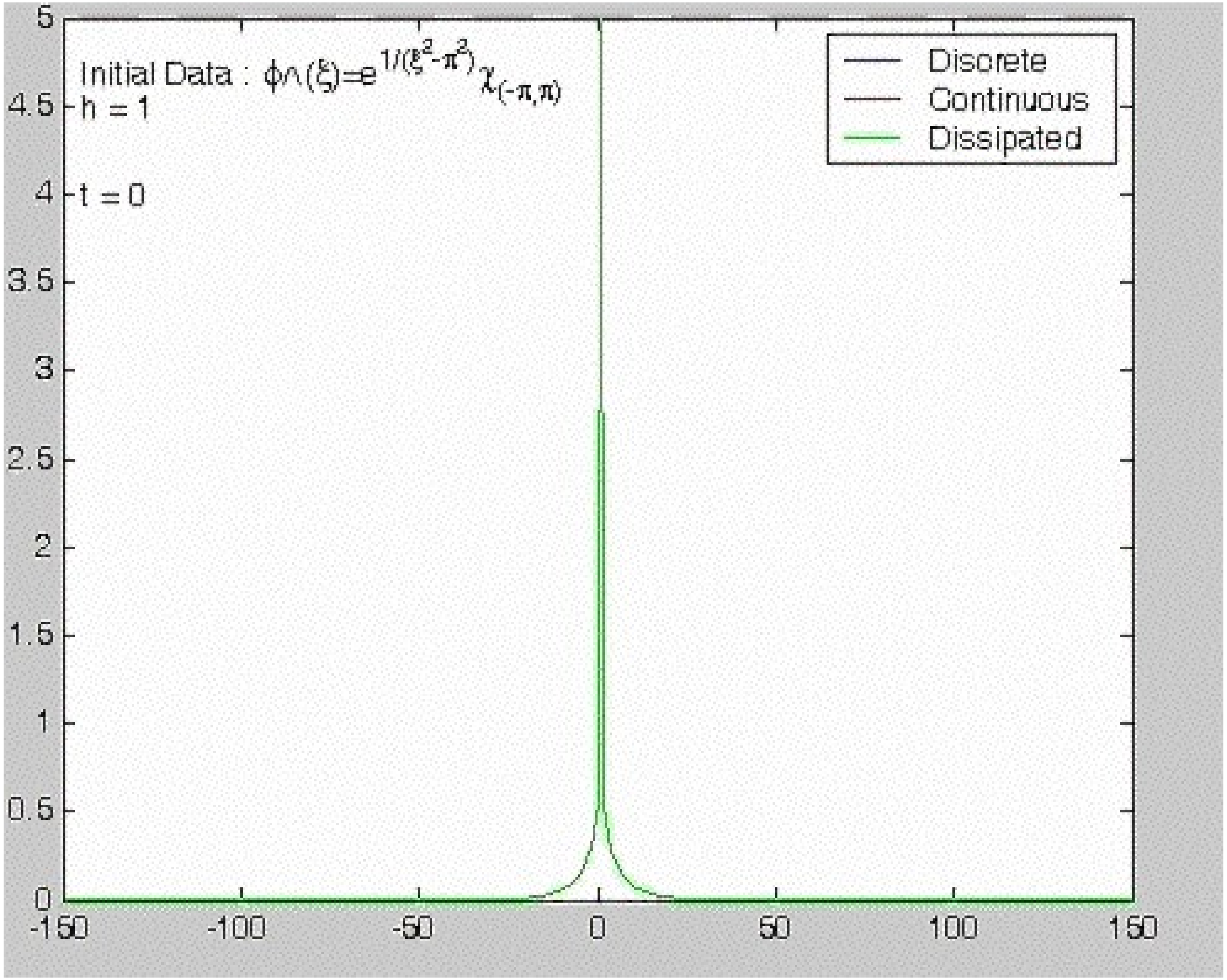
For $q = 2$, $s = \frac{1}{2}\left(\frac{1}{\alpha} - 1\right)$. Adding numerical viscosity at a suitable scale we can reach the H^s-regularization for all $s < 1/2$, but not for the optimal case $s = 1/2$. This will be a limitation to deal with the critical nonlinearities. Indeed, when $\alpha = 1/2$,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

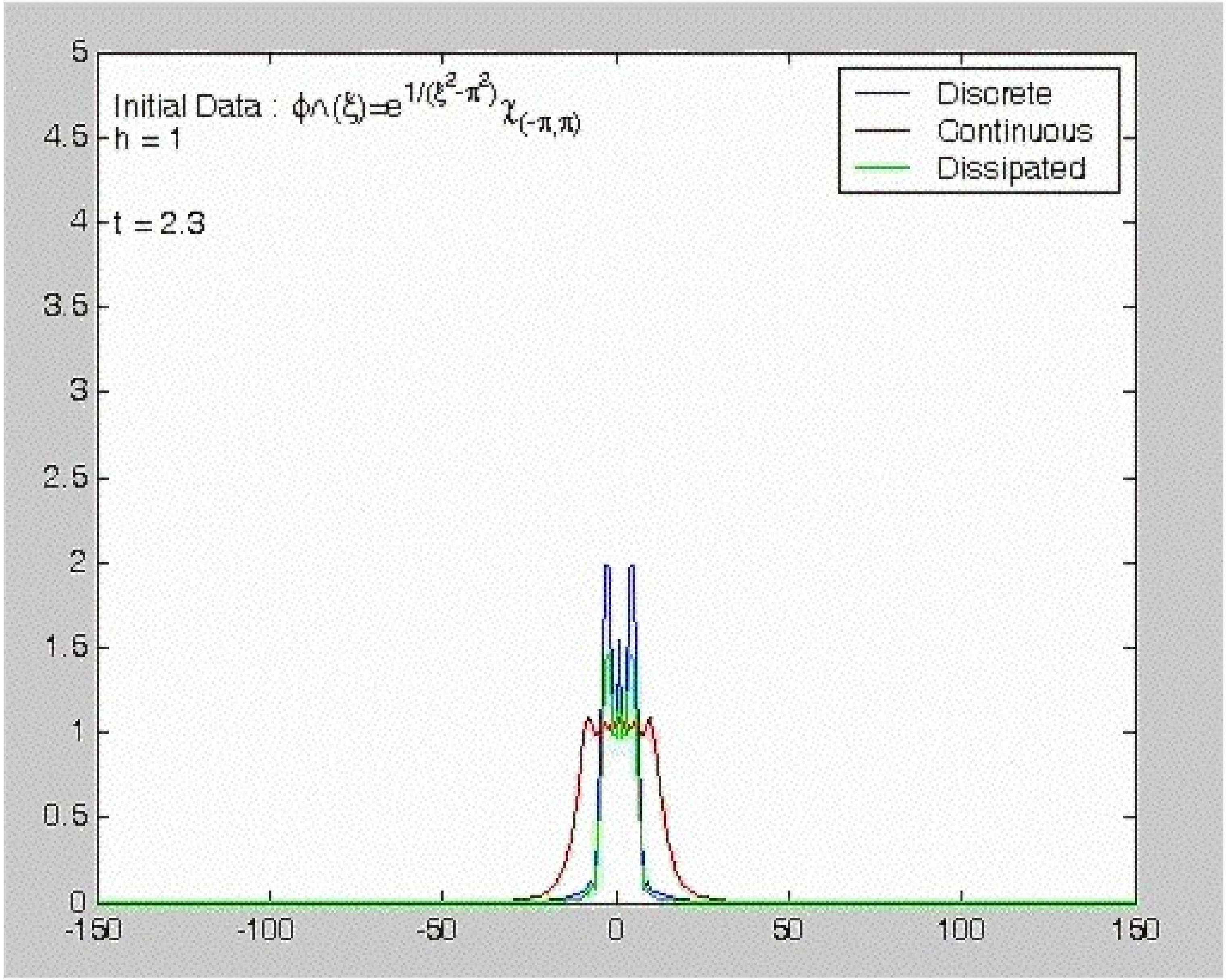
The proof of these results relies on the principle above. Solutions are obtained as an iterated convolution of a discrete Schrödinger Kernel and a parabolic one. The heat kernel kills the high frequencies, while for the low ones the discrete Schrödinger kernel behaves very much the same as the continuous one.

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

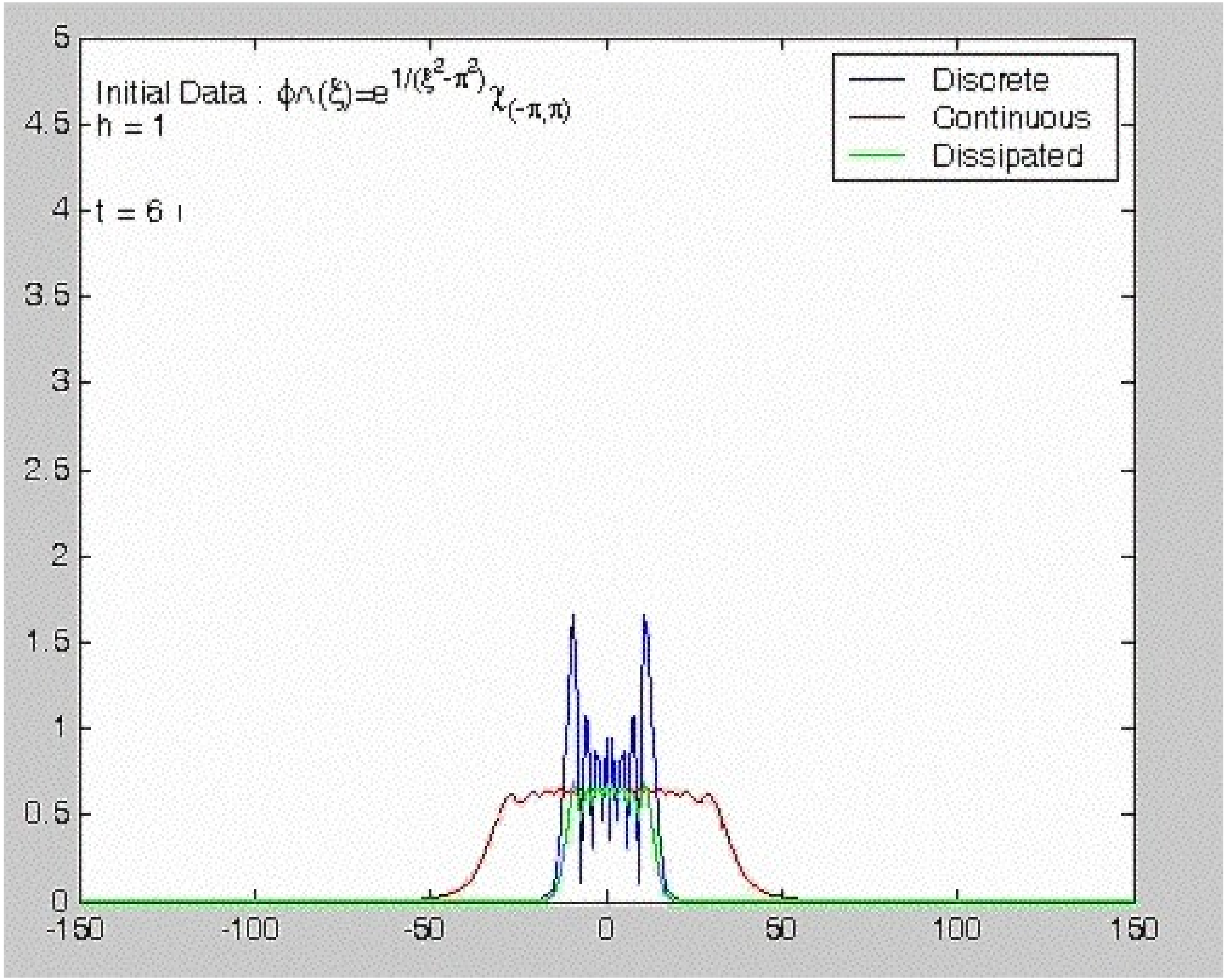


L^∞ norm decay
Initial Data : φ∧(ξ)=e^{1/((ξ-π/2)^2-1)}χ_(π/2-1,π/2+1)
h=1
Discrete
Continuous
Dissipated
Two Grid
0
0.1
0.2
0.3
0.4
0.5
5
10
15
20
25
30
t

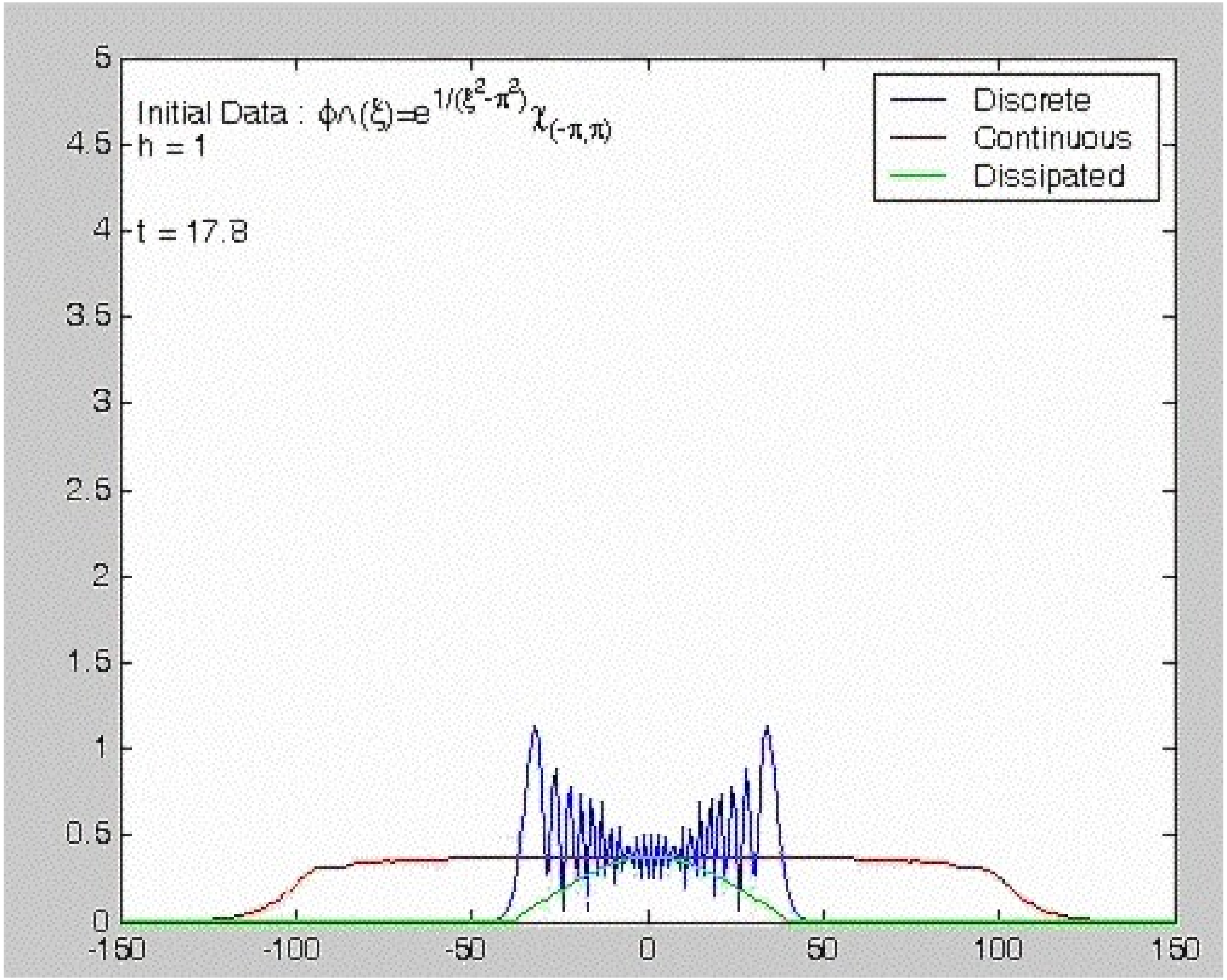

Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 0
Discrete
Continuous
Dissipated
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-150
-100
-50
0
50
100
150



Initial Data : φ^(ξ)=e^{1/(ξ²-π²)} χ_(-π,π)
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 : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 6
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 = 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:

$$\left\{ \begin{array}{rcll} iu_t + u_{xx} & = & |u|^p u & x \in \mathbf{R}, t > 0, \\ u(0,x) & = & \varphi(x) & x \in \mathbf{R}, \end{array} \right. \tag{10}$$

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

$$u(t) = S(t)\varphi - i\int_0^t S(t-s)|u(s)|^p u(s)ds, \tag{11}$$

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:

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h &= ia(h)\Delta_h u^h + |u^h|^p u^h, \qquad t > 0 \\ u^h(0) &= \varphi^h, \\ i\dfrac{du^h}{dt} + \Delta_h u^h &= -ia(h)\Delta_h u^h + |u^h|^p u^h, \quad t < 0. \end{cases} \tag{12}$$

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:

- *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 $h \longrightarrow 0$.*

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 .

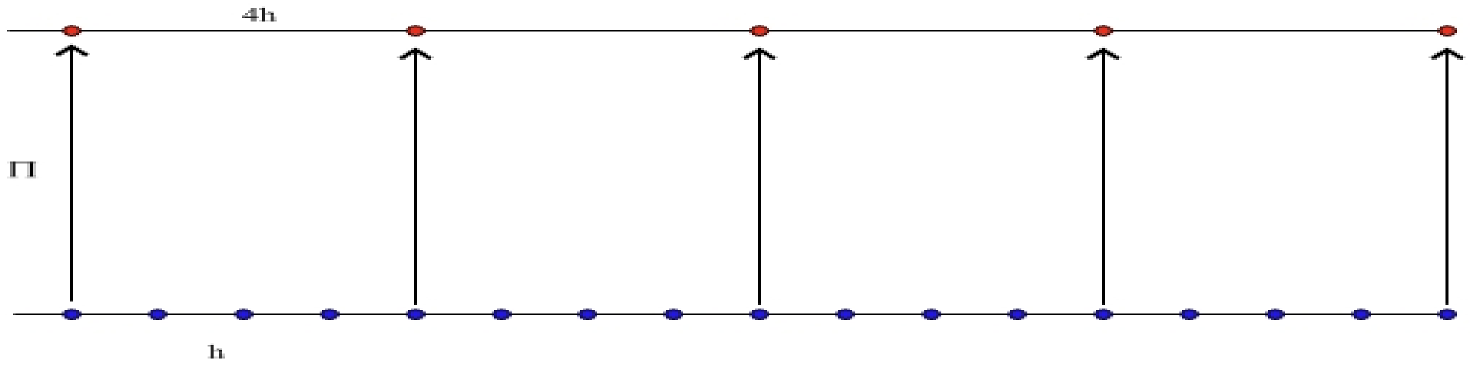
The idea: To work on the grid of mesh-size h with slowly oscillating data interpolated from a coarser grip of size $4h$. The ratio $1/2$ of meshes does not suffice!

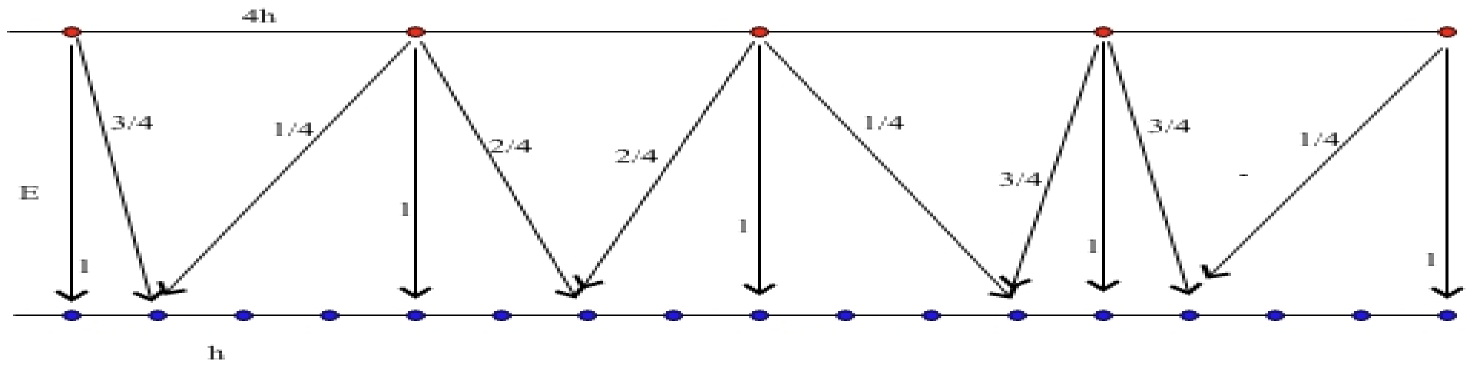
The space of discrete functions on the coarse mesh $4h\mathbf{Z}$:

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

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
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 $\Pi : \mathbb{C}^{h\mathbf{Z}} \to \mathbb{C}_4^{h\mathbf{Z}}$:

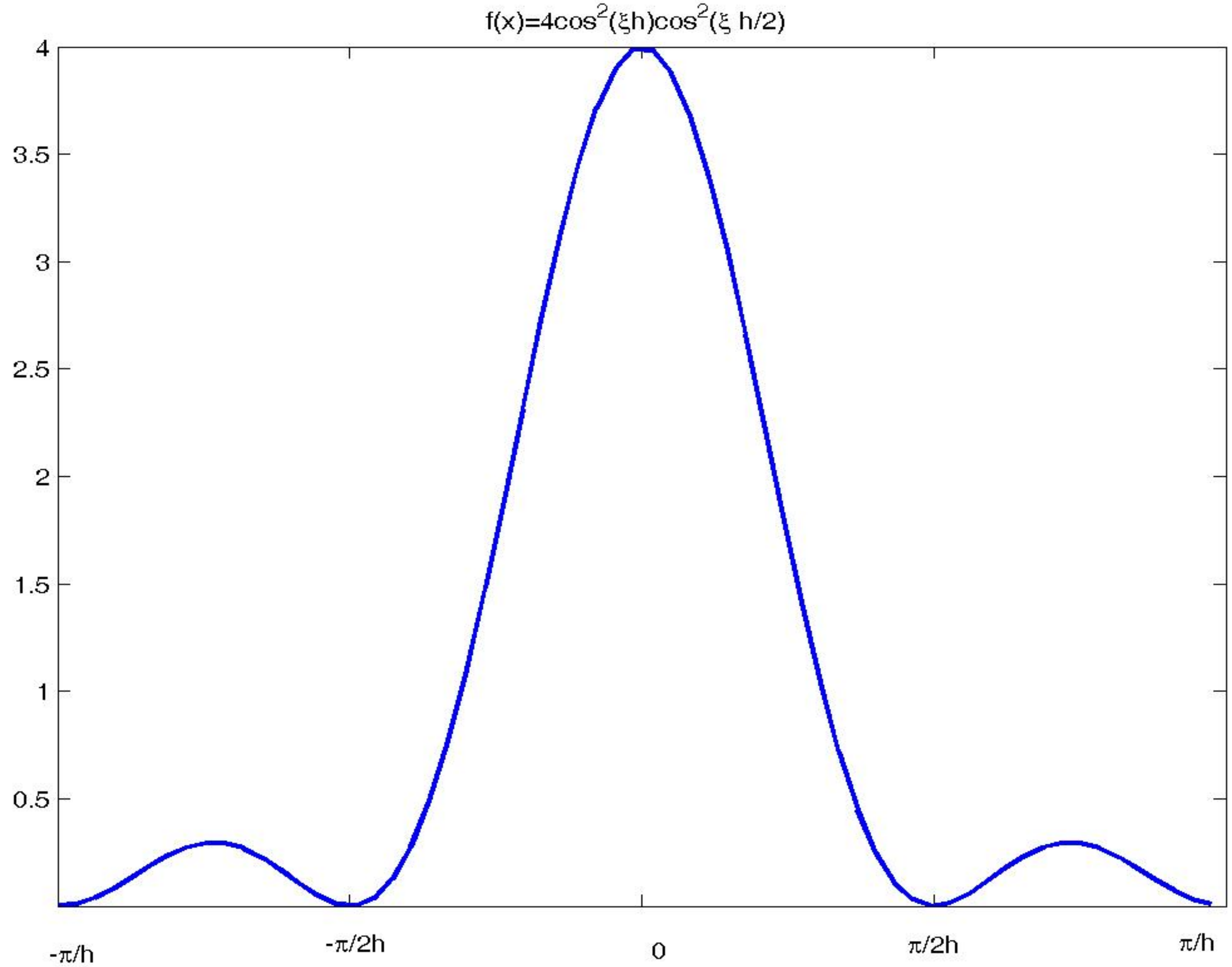
$$(\Pi\phi)((4j+r)h) = \phi((4j+r)h)\delta_{4r}, \forall j \in \mathbf{Z}, r = \overline{0,3}, \phi \in \mathbb{C}^{h\mathbf{Z}}.$$

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:

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


f(x)=4cos2(ξh)cos2(ξ h/2)
4
3.5
3
2.5
2
1.5
1
0.5
-π/h
-π/2h
0
π/2h
π/h

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),

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

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.*

SOS vanish at the spectral points $\pm\pi/2h$ *implies gain of integrability.*

This is consistent with the previous analysis of the viscosity method.

Concerning the local smoothing properties we can prove that

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

$$\sup_{j\in\mathbf{Z}} \int_{-\infty}^{\infty} \left|(D^{1-1/r} e^{it\Delta_h} \tilde{\Pi} f)_j\right|^2 dt \lesssim \left|\tilde{\Pi} f\right|^2_{l^r(h\mathbf{Z})} \tag{13}$$

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

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

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

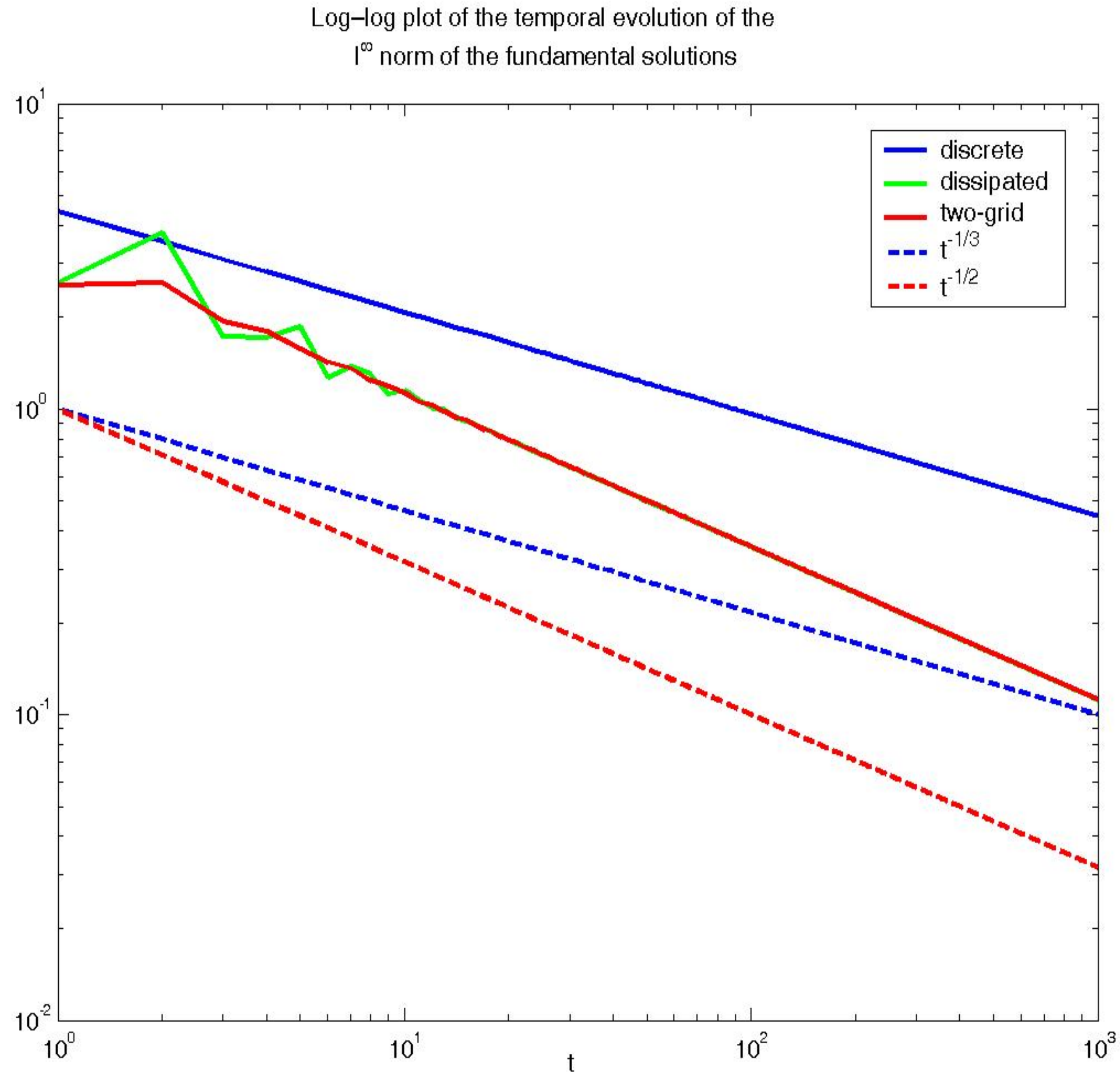
Then, using the fact that $\cos^4 \xi \cos^4(\xi/2)$ vanishes at $\xi = \pm\pi$, we can compensate the singularity of $\sin(\xi)$ in the denominator and *guarantee that*

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

SOS vanish at the spectral points $= \pm\pi$*, implies gain of local regularity.*

This is also consistent with the results obtained by means of the viscosity method.

The effect of the two-grid algorith combining the meshes h *and* $4h$ *is clearly observed when trying to mimic at the discrete level the properties of the continuous semigroup.*



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

A TWO-GRID CONSERVATIVE APPROXIMATION OF THE NLSE

Consider the semi-discretization

$$i\frac{du^h}{dt} + \Delta_h u^h = \widetilde{\Pi} f(u^h),\ t \in \mathbb{R}; \qquad u^h(0) = \widetilde{\Pi}\varphi^h, \qquad (14)$$

where $f(u^h)$ *is a suitable approximation of* $|u|^p u$ *with* $0 < p < 4$.

By using the two-grid filtering operator both in the nonlinearity and on the initial data we guarantee that the corresponding trajectories enjoy the properties above of gain of local regularity and integrability.

But to prove the stability of the scheme we need to guarantee the conservation of the $l^2(h\mathbf{Z})$ *norm of solutions, a property that the* *solutions of NLSE satisfy. For that the nonlinear term* $f(u^h)$ *has to be chosen such that* $(\widetilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})} \in \mathbb{R}$. *These property is guranteed with the choice*

$$(f(u^h))_{4j} = g\left((u^h_{4j} + \sum_{r=1}^{3} \frac{4-r}{4}(u^h_{4j+r} + u^h_{4j-r}))\Big/4\right); \quad g(s) = |s|^p s.$$

The same arguments as in the viscosity method allow showing that the solutions of the two-grid numerical scheme converge as $h \to 0$ *to the solutions of the continuous NLSE.*

TWO GOOD NEWS:

- *Lecture is ending.... ;*
- *Things improve when we also discretize in time.*

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

CONCLUSIONS:

- FOURIER FILTERING (AND SOME OTHER VARIANTS LIKE NUMERICAL VISCOSITY,...) ALLOW BUILDING NUMERICAL SCHEMES FOR AN EFFICIENT APPROXIMATION OF LINEAR AND NONLINEAR SCHÖDINGER EQUATIONS.

- 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. 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, 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!

L. Ignat and E. Z. C. R. Acad. Sci. Paris, **340** *(7) (2005), 529534.*

Theorem 8 *(Global well-posedness of the numerical problem)* *Let* $p \in (0,4)$ *and* $\alpha(h) \in (1/2, 2/p]$. *Let* $q(h)$ *be such that* $(q(h), p+2)$ *is an* $\alpha(h)$*-admissible pair.*

Then for every $\varphi^h \in l_h^2(\mathbf{Z})$, *there exists a unique global solution*

$$u^h \in C([0,\infty), l_h^2(\mathbf{Z})) \cap \mathbf{L}_{\mathbf{loc}}^{\mathbf{q(h)}}([\mathbf{0},\infty); \mathbf{l}_{\mathbf{h}}^{\mathbf{p+2}}(\mathbf{Z})) \tag{15}$$

of the problem (12) which satisfies the following estimates

$$||u^h||_{L^\infty([0,\infty), l_h^2(\mathbf{Z}))} \leq ||\varphi||_{l_h^2(\mathbf{Z})} \tag{16}$$

and

$$||u^h||_{L^{q(h)}(I, l_h^{p+2}(\mathbf{Z}))} \leq c(I)||\varphi||_{l_h^2(\mathbf{Z})} \tag{17}$$

where the above constants are independent of h.

Theorem 9 *(Convergence as $h \to 0$)*

The sequence Eu^h satisfies

$$Eu^h \overset{\star}{\rightharpoonup} u \text{ in } L^\infty([0,\infty), L^2(\mathbf{R})), \tag{18}$$

$$Eu^h \rightharpoonup u \text{ in } L^s_{loc}([0,\infty), L^{p+2}(\mathbf{R})), \forall\, s < q, \tag{19}$$

$$Eu^h \to u \text{ in } L^2_{loc}([0,\infty) \times \mathbf{R}), \tag{20}$$

$$|Eu^h|^p |Eu^h| \rightharpoonup |u|^p u \text{ in } L^{q'}_{loc}([0,\infty), L^{(p+2)'}(\mathbf{R})) \tag{21}$$

where u is the unique weak solution of (NSE).