# Dispersive numerical schemes for Schrödinger equations

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To build convergent numerical schemes for nonlinear PDE of dispersive type: SCHRÖDINGER EQUATION.
Similar problems for other dispersive equations: Korteweg-de-Vries, wave equation, ...

Goal: To cover the classes of NONLINEAR 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, Kato, Ginibre, Velo, Cazenave, Weissler, Saut, Bourgain, Kenig, Ponce, Saut, Vega, Koch, Tataru, Burq, Gérard, Tzvetkov, ...)

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.

For this we need to adapt at the discrete numerical level the techniques developed in the continuous context.

WARNING!

NUMERICS = CONTINUUM + (POSSIBLY) SPURIOUS

Note that the appropriate functional setting often depends on the PDE on a subtle manner.
Consider for instance:

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

$A$ 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 $f : H \to H$ 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 $p > 1$.

Then, one needs to discover other properties of the underlying linear equation (smoothing, dispersion): IF $e^{At}u_0 \in X$, then 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 check 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.

IF WORKING IN $C([0,T];: H) \cap X$ IS NEEDED FOR SOLVING THE PDE, FOR PROVING CONVERGENCE OF A NUMERICAL SCHEME WE WILL NEED TO MAKE SURE THAT IT FULFILLS SIMILAR STABILITY PROPERTIES IN $X$ (OR $X_h$).

THIS OFTEN FAILS!

Consider the Linear Schrödinger Equation (LSE):

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

It may be written in the abstract form:

$$u_t = Au, \quad A = i\Delta = i\partial^2 \cdot /\partial x^2.$$

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.

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

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

- Local gain of $1/2$-derivative: If the initial datum $\varphi$ 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 and compactness results for nonlinear Schrödinger equations (NLS).

The same convergence result holds for semilinear equations

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

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 continuous 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?

The following is well-known for the NSE:

$$\begin{cases} iu_t + u_{xx} = |u|^p u & x \in \mathbf{R}, t > 0, \\ u(0,x) = \varphi(x) & x \in \mathbf{R}. \end{cases} \tag{2}$$

**Theorem**

*( Global existence in $L^2$, Tsutsumi, 1987). For $0 \le p < 4$ 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 $L^2$.*

This result can not be proved by methods based purely on energy arguments.

## The three-point finite-difference scheme

Consider the finite difference approximation

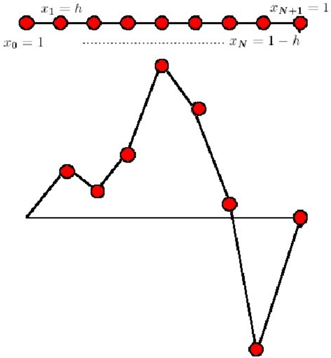
$$i\frac{du^h}{dt} + \Delta_h u^h = 0, t \neq 0, \quad u^h(0) = \varphi^h. \tag{3}$$

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 $t \geq 0$.



## LACK OF DISPERSION OF THE NUMERICAL SCHEME

Consider the semi-discrete Fourier Transform

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

There are "slight" but important differences between the symbols of the operators $\Delta$ and $\Delta_h$:

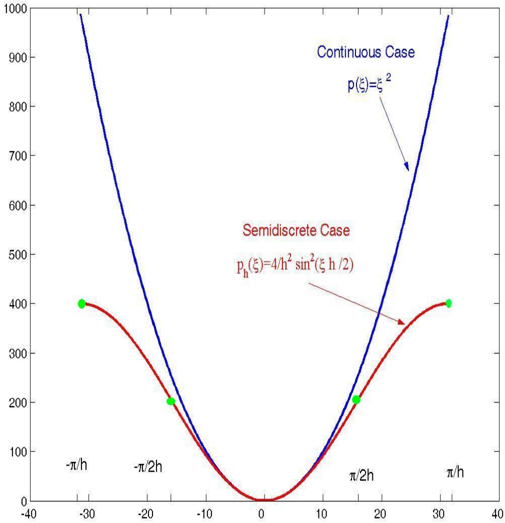
$$p(\xi) = -\xi^2, \, \xi \in \mathbf{R}; \quad p_h(\xi) = -\frac{4}{h^2} \sin^2(\frac{\xi h}{2}), \, \xi \in [-\frac{\pi}{h}, \frac{\pi}{h}].$$

For a fixed frequency $\xi$, 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.

The main differences are:

- $p(\xi)$ is a convex function; $p_h(\xi)$ changes 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 of the numerical scheme and consequently, make the scheme useless for nonlinear problems.



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

LACK OF CONVEXITY = LACK OF INTEGRABILITY GAIN.

The symbol $p_h(\xi)$ looses convexity near $\pm\pi/2h$. Applying the stationary phase lemma (G. Gigante, F. Soria, IMRN, 2002):

**Theorem**

*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.

Independent work on the Schrödinger equation in lattices:

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

L. Giannoulis, M. Herrmann & A. Mielke, Multiscale volume, 2006.

It is shown that the fundamental solution on the discrete lattice decays in $L^\infty$ as $t^{-1/3}$ and not as $t^{-1/2}$ as in the continuous frame.

**Lemma**

*(Van der Corput)*
*Suppose $\phi$ 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 LOCAL REGULARITY GAIN.

**Theorem**

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

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

Initial data whose Fourier transform is concentrated around $\pi/h$.

LACK OF SLOPE= VANISHING GROUP VELOCITY.

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

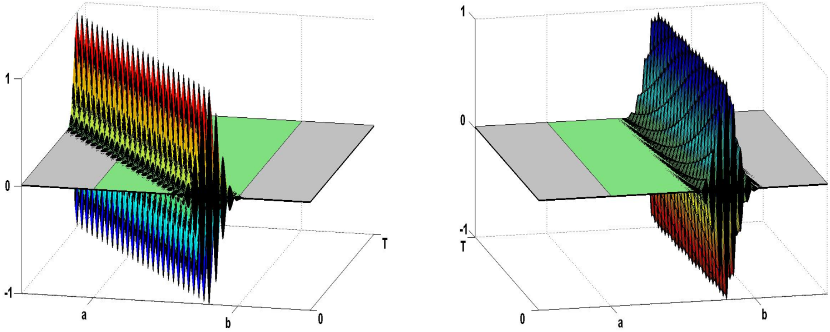



Figure: Localized waves travelling at velocity $= 1$ for the continuous equation (left) and wave packet travelling at very low group velocity for the FD scheme (right).

## A REMEDY: FOURIER FILTERING

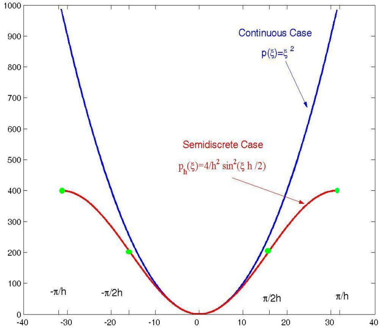
Eliminate the pathologies that are concentrated on the points $\pm\pi/2h$ and $\pm\pi/h$ of the spectrum, i. e. replace the complete solution

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

by the filtered one

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

This guarantees the same dispersion properties of the continuous Schrödinger equation to be uniformly (on $h$) true together with the convergence of the filtered numerical scheme.



But Fourier filtering:

- Is computationally expensive: Compute the complete solution in the numerical mesh, compute its Fourier transform, 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:

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

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

$$a(h) \to 0$$

as $h \to 0$.

This condition guarantess the consistency with the LSE.

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).
- It is natural also from a mechanical point of view: elasticity $\rightarrow$ viscoelasticity.

The main dispersive properties of this scheme are as follows:

**Theorem**

*($L^p$-decay) Let us 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*

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

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

## Theorem

*(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*

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

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

For $q = 2$, $s = (1/\alpha - 1)/2$. 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 critical nonlinearities. Indeed, when $\alpha = 1/2$, $a(h) = 1$ and the scheme is no longer an approximation of the Schrödinger equation itself.

Sketch of the proof:

- 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 continuous dispersive and sharp estimates of Bessel functions arising in the explicit form of the discrete heat kernel (Kenig-Ponce-Vega, Barceló-Córdoba,...).

# NUMERICAL APPROXIMATION OF THE NLSE

The lack of dispersive properties of the conservative linear scheme indicates it is hard to use for solving nonlinear problems. But, in fact, explicit travelling wave solutions for

$$i\frac{du^h}{dt} + \Delta_h u^h = |u_j^h|^2(u_{j+1}^h + u_{j-1}^h),$$

show that this nonlinear discrete model does not have any further integrability property (uniformly on $h$) other than the trivial $L^2$-estimate (M. J. Ablowitz & J. F. Ladik, J. Math. Phys., 1975.)

Consider now the NSE:

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

According to Tsutsumi's result (1987) the equation is well-posed in $C(\mathbf{R}, L^2(\mathbf{R})) \cap L^q_{loc}(L^{p+2})$ with $q = 4(p+1)/p$ for $0 \leq p < 4$ and $\varphi \in L^2(\mathbf{R})$.

Consider now the semi-discretization:

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

with $a(h) = h^{2-\frac{1}{\alpha(h)}}$ 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 $h \to 0$.

# Drawbacks:

- The viscoity has to be tunned depending on the exponent in the nonlinearity
- Solutions could decay too fast as $t \to \infty$ due to the viscous effect.

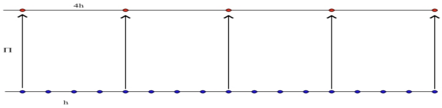
# TWO-GRID ALGORITHM: DO NOT MODIFY THE SCHEME BUT SIMPLY PRECONDITION THE INITIAL DATA!

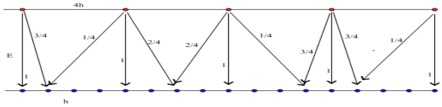
Let $V_4^h$ be the space of slowly oscillating sequences (SOS) on the fine grid

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

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

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



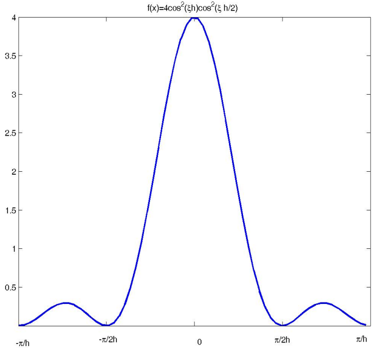



We now define the smoothing operator

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

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:

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



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

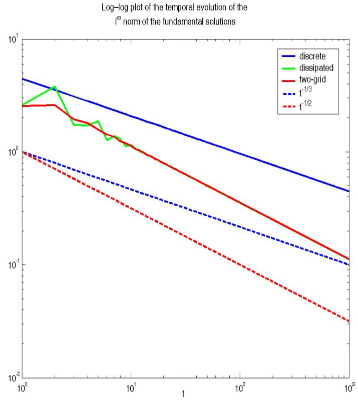
**Theorem**

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

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

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

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


Log–log plot of the temporal evolution of the
$l^\infty$ 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

# A TWO-GRID CONSERVATIVE APPROXIMATION OF THE NLSE

Consider the semi-discretization

$$i\frac{du^h}{dt} + \Delta_h u^h = |\widetilde{\Pi}^*(u^h)|^p\, \widetilde{\Pi}^*(u^h),\ t \in \mathbf{R}; u^h(0) = \varphi^h,$$

with $0 < p < 4$.

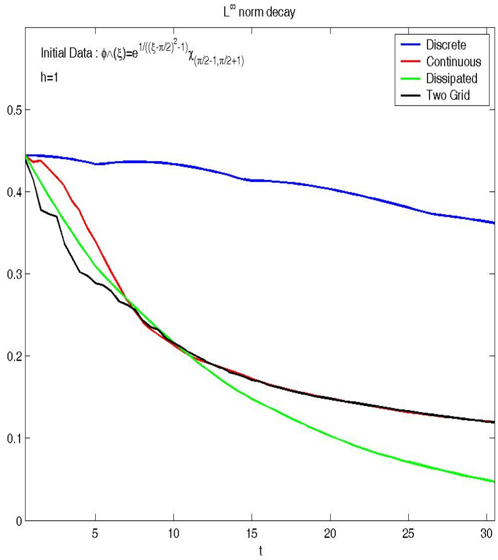
By using the two-grid filtering operator $\widetilde{\Pi}$ both in the nonlinearity and on the initial data we guarantee that the corresponding trajectories enjoy the properties above of gain of local regularity and integrability.

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

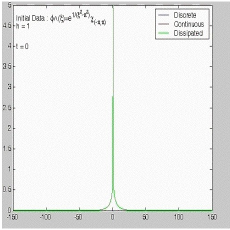
$$(\widetilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})} \in \mathbf{R}.$$

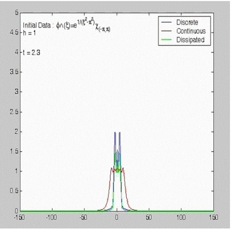
This property is guaranteed with the choice

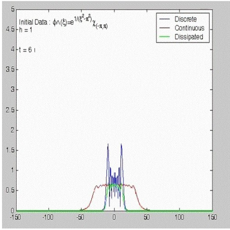
$$f(u^h) = |\widetilde{\Pi}^*(u^h)|^p\, \widetilde{\Pi}^*(u^h)$$

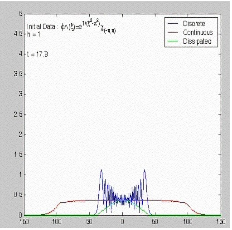


L∞ norm decay
Initial Data : φ∧(ξ)=e^{1/((ξ-π/2)^2-1)} χ_(π/2-1,π/2+1)
h=1
Discrete
Continuous
Dissipated
Two Grid
0.5
0.4
0.3
0.2
0.1
0
5
10
15
20
25
30
t


Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 0
Discrete
Continuous
Dissipated


Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 2.3
Discrete
Continuous
Dissipated


Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 6
Discrete
Continuous
Dissipated


Initial Data : $\phi\wedge(\xi)=e^{1/(\xi^2-\pi^2)}\chi_{(-\pi,\pi)}$
h = 1
t = 17.8
Discrete
Continuous
Dissipated

Is all this analysis needed?
In practice, we could:

- 1.- Approximate the initial data $\varphi$ by smooth ones
- 2.- Use standard tools of numerical analysis for smooth data that allow handeling stronger nonlinearities because the corresponding solutions are bounded.
- 3.- By this double approximation derive a family of numerical solutions converging to te continuous one.

Warning! When doing that we pay a lot (!!!) at the level of the orders of convergence...

An example: The two-grid method yields:

$$||u^h - \mathcal{T}^h u||_{L^\infty(0,T;\ell^2(h\mathbf{Z}))} \leq C(T, ||\varphi||_{H^s})h^{s/2}.$$

When using the standard $5$-point scheme, without dispersive estimates, we can regularize the $H^s$ data by a $H^1$ approximation and then use that the solutions of the Schrödinger equation are in $L^\infty$ to handle the nonlinearity. When this is done we get an order of convergence of $|\log h|^{-s/(1-s)}$ instead of $h^s/2$.

This is due to the following threshold for the aproximation process:

**Lemma**

*Let $0 < s < 1$ and $h \in (0,1)$. Then for any $\varphi \in H^s(\mathbf{R})$ the functional $J_{h,\varphi}$ defined by*

$$J_{h,\varphi}(g) = \frac{1}{2}\|\varphi - g\|^2_{L^2(\mathbf{R})} + \frac{h}{2}\exp(\|g\|^2_{H^1(\mathbf{R})}) \tag{12}$$

*satisfies:*

$$\min_{g \in H^1(\mathbf{R})} J_{h,\varphi}(g) \le C(\|\varphi\|_{H^s(\mathbf{R})}, s)|\log h|^{-s/(1-s)}. \tag{13}$$

*Moreover, the above estimate is optimal.*

# Drawbacks:

- We need a fine choice of the grid ratio to make sure the pathological frequencies are damped out.

Extensive literature: Reed, W.H. & Hill, 1973; Arnold, D.N., 1979; Cockburn B., Shu C-W, 90's ; Arnold D.N., Brezzi F., Cockburn B., Marini D. 2000 - 2002, M. Ainsworth 2004,...

We consider the simplest version for the 1D Schrödinger equation in a uniform grid of size $h > 0$: $x_i = hi$.

Deformations are now piecewise linear but not necessarily continuous on the mesh points:

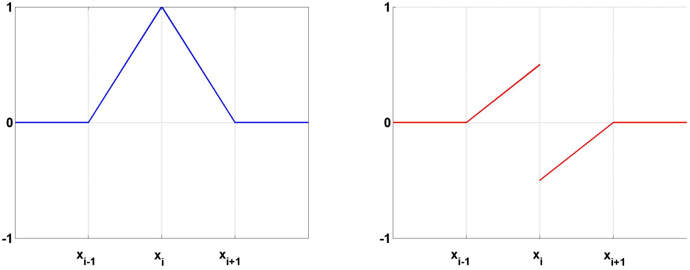



Figure: Basis funtions: $\phi_i$ (left) and $\widetilde{\phi}_i$ (right)

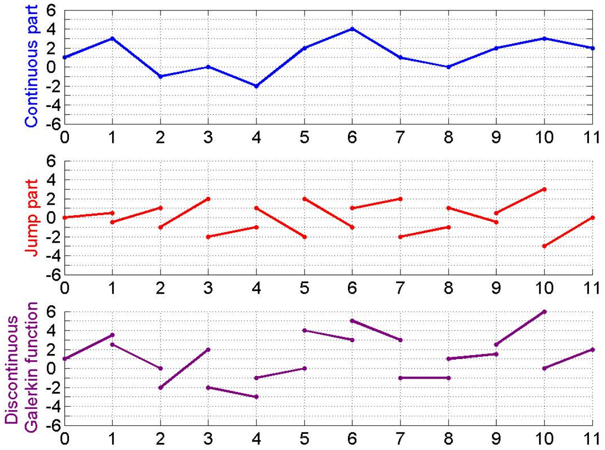



Figure: Decomposition of a DG defomration into its continuous and jump components.

# Variational formulation

Relevant notation:

- Average: $\{f\}(x_i) = \frac{f(x_i+)+f(x_i-)}{2}$
- Jump: $[f](x_i) = f(x_i-) - f(x_i+)$
- $V_h = \{v \in L^2(\mathbf{R}) \big| v|_{(x_j,x_{j+1})} \in P_1, \|v\|_h < \infty\}$,
- $\|v\|_h^2 = \sum_{j\in\mathbf{Z}} \int_{x_j}^{x_{j+1}} |v_x|^2\,dx + \frac{1}{h}\sum_{j\in\mathbf{Z}} [v]^2(x_j)$

The bilinear form and the DG Cauchy problem:

$$\begin{aligned} a_h^s(u,v) &= \sum_{j\in\mathbf{Z}} \int_{x_j}^{x_{j+1}} u_x v_x\,dx - \sum_{j\in\mathbf{Z}} ([u](x_j)\{v_x\}(x_j) + [v](x_j)\{u_x\}(x_j)) \\ &+ \frac{s}{h}\sum_{j\in\mathbf{Z}} [u](x_j)[v](x_j), \; s>0 \text{ is a penalty parameter.} \end{aligned}$$

$$\begin{cases} u_h^s(x,t) \in V_h, t>0 \\ i\frac{d}{dt}\int_{\mathbf{R}} u_h^s(x,t)v(x)\,dx + a_h^s(u_h^s(\cdot,t),v) = 0, \forall v \in V_h, \\ u_h^s(x,0) = u_h^0(x). \end{cases} \tag{14}$$

# DG as a system of ODE's

Decompose solutions into the FE+jump components:

$$u_h^s(x,t) = \sum_{j\in\mathbf{Z}} u_j(t)\phi_j(x) + \sum_{j\in\mathbf{Z}} \widetilde{u}_j(t)\widetilde{\phi}_j(x).$$

Then $U_h^s(t) = (u_j(t), \widetilde{u}_j(t))'_{j\in\mathbf{Z}}$ solves the system of ODE's:

$$iM_h\dot{U}_h^s(t) = R_h^s U_h^s.$$

$M_h$: mass matrix, $R_h^s$ -rigidity matrix (symmetric, bloc tri-diagonal)

Applying the Fourier transform

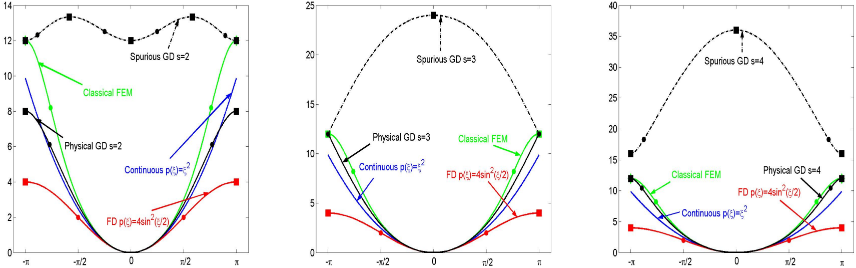
$$i\begin{pmatrix} \widehat{u}_t^h(\xi,t) \\ \widehat{\widetilde{u}}_t^h(\xi,t) \end{pmatrix} = -A_h^s(\xi)\begin{pmatrix} \widehat{u}^h(\xi,t) \\ \widehat{\widetilde{u}}^h(\xi,t) \end{pmatrix}. \tag{15}$$

The eigenvalues of $A_h^s(\xi)$ constitute two branches

$$\begin{cases} \Lambda_{p,h}^s(\xi) = \left(\lambda_{p,h}^s(\xi)\right)^2 & \text{(physical dispersion)} \\ \Lambda_{s,h}^s(\xi) = \left(\lambda_{s,h}^s(\xi)\right)^2 & \text{(spurious dispersion)} \end{cases}$$

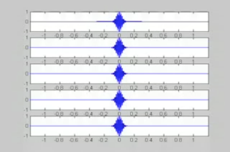
The corresponding eigenvectors have the energy polarized either in the FE subspace (physical solutions) or in the jump subspace (spurious solutions).

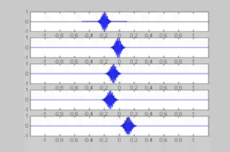
# Branches of eigenvalues for different values of $s$

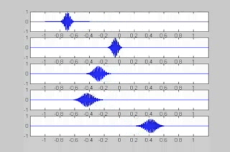



The viscous approach will work while the two-grid one will hardly do it because of the uncertain location of the pathological points in dispersion curves.

# Gaussian races







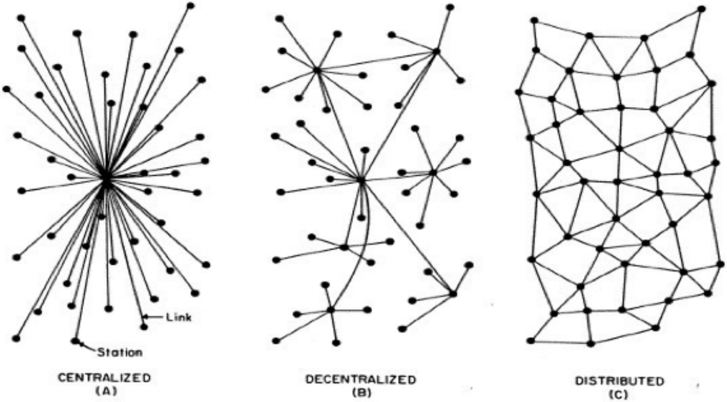



FIG. I — Centralized, Decentralized and Distributed Networks

1. Motivation
2. Dispersion for the $1-d$ Schrödinger equation
3. Lack of numerical dispersion
4. Remedies
   - Fourier filtering
   - Numerical viscosity
   - A bigrid algorithm
5. Orders of convergence
6. DG methods
7. Networks
8. Conclusions & References

# Conclusions

- Fourier filtering and some other variants (numerical viscosity, two-grid filtering,...) allow building efficient numerical schemes for linear and nonlinear Schrödinger equation: widder classes of nonlinearities, better convergence rates for rough data,...
- A systematic analysis of their computational efficiency is to be done.
- Both numerical viscosity and two-grids have drawbacks related to the tunning of parameters.
- Discontinuous Galerkin methods present added technical difficulties related to the spurious branch of waves.
- Much remains to be done to be develop a complete theory (multi-d, variable coefficients,...) and it should combine fine tools from harmonic analysis, PDE and Numerics.
- Extensions to networks is widely open both in the continuous and discrete setting.

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¡Thank you!

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