Dispersive numerical schemes for Schrödinger equations

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Content

To build convergent numerical schemes for NONLINEAR SCHRÖDINGER EQUATIONS (NSE)

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

Key point: This has been done succesfully for the PDE models: (Strichartz, Kato, Ginibre, Velo, Cazenave, Weissler, Saut, Bourgain, Kenig, Ponce, Saut, Vega, Koch, Tataru, Burq, Gérard, Tzvetkov, ...)

What about Numerical schemes?

FROM FINITE TO INFINITE DIMENSIONS IN PURELY CONSERVATIVE SYSTEMS.....
WITH OR WITHOUT DISSIPATION?

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.

In that frame, numerical schemes need to reproduce at the discrete level similar properties.

But the most classical ones often fail to do it!

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 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 and compactness results for nonlinear Schrödinger equations (NLS).

The following is well-known for the NSE:

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

Theorem

(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.

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

The three-point finite-difference scheme

Consider the finite difference approximation

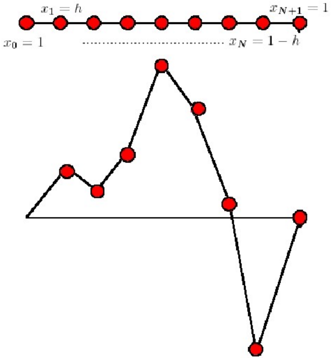
$$i\frac{du^h}{dt} + \Delta_h u^h = 0, t \neq 0, \quad u^h(0) = \varphi^h. \tag{2}$$

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 $t \geq 0$.



LACK OF DISPERSION OF THE NUMERICAL SCHEME

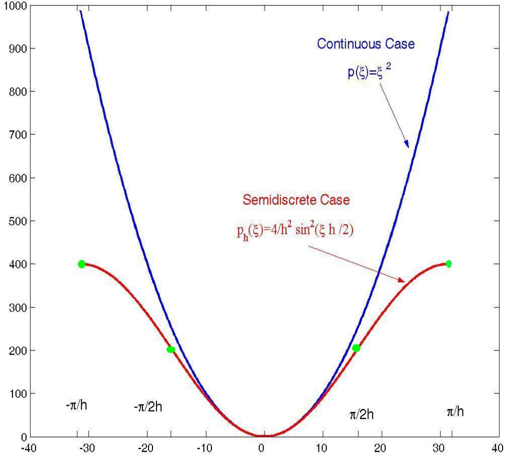
Consider the semi-discrete Fourier Transform

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

There are "slight" but important differences between the symbols of the operators 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.



Lack of coherence?

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.

This can be seen using classical results on the asymptotic behavior of oscillatory integrals:

Lemma

(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

$$\left| \int_a^b e^{it\phi(\xi)} d\xi \right| \leq c_k t^{-1/k} \tag{3}$$

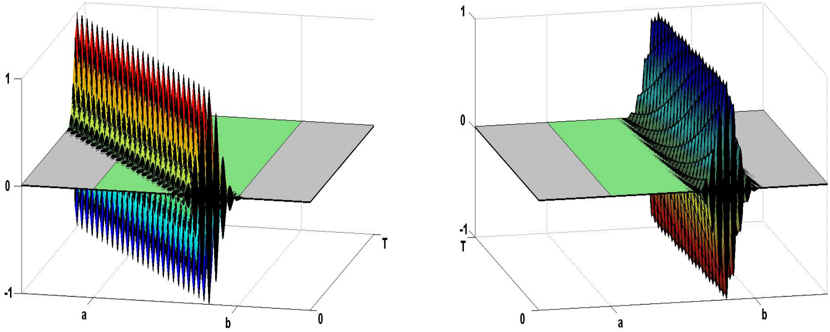


Figure: Localized waves travelling at velocity $= 1$ for the continuous equation (left) and wave packet travelling at very low group velocity for the FD scheme (right).

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.)

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

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

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:

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = ia(h)\Delta_h u^h, & t > 0, \\ u^h(0) = \varphi^h, \end{cases} \tag{4}$$

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 $t > 0$:

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

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 $a(h)$.

- 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 viscosity 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.

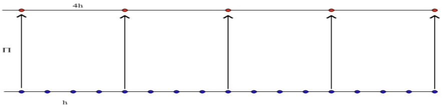
THE TWO-GRID ALGORITHM: DO NOT MODIFY THE SCHEME BUT SIMPLY PRECONDITION THE INITIAL DATA!

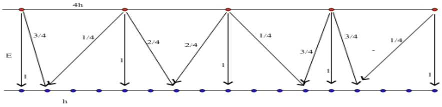
Let V_4^h be the space of slowly oscillating sequences (SOS) on the fine grid

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

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

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



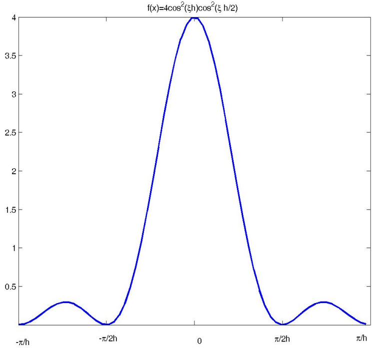


We now define the smoothing operator

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

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),

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

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

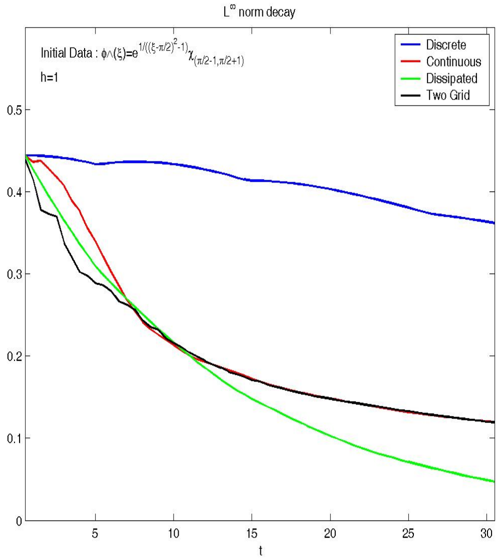
$$(\widetilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})} \in \mathbf{R}.$$

This property is guaranteed with the choice

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

Drawbacks:

- The space of two-grid data is not time-invariant. The data have to be adjusted after a finite T: $[0, T]$, $[T, 2T]$,....
- Succes depends on the identification of the location of pathological frequencies and the choice of a srategic value for the mesh-ratio.


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

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

- 1.- Approximate the initial data φ 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^∞ 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

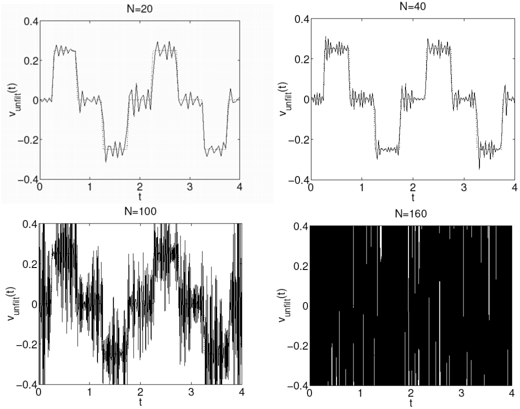
Let $0 < s < 1$ and $h \in (0,1)$. Then for any $\varphi \in H^s(\mathbf{R})$ the functional $J_{h,\varphi}$ defined by

$$J_{h,\varphi}(g) = \frac{1}{2}\|\varphi - g\|^2_{L^2(\mathbf{R})} + \frac{h}{2}\exp(\|g\|^2_{H^1(\mathbf{R})}) \tag{5}$$

satisfies:

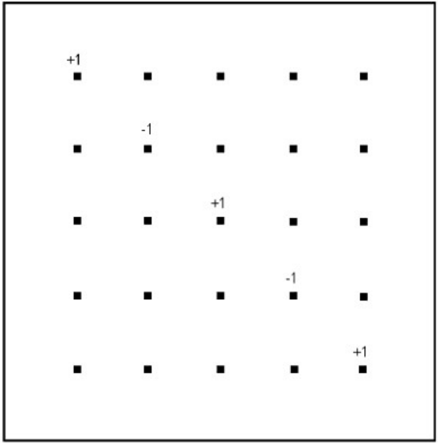
$$\min_{g \in H^1(\mathbf{R})} J_{h,\varphi}(g) \le C(\|\varphi\|_{H^s(\mathbf{R})}, s)|\log h|^{-s/(1-s)}. \tag{6}$$

Moreover, the above estimate is optimal.



The control diverges as $h \to 0$.

About the discussion on infinite dimensional versus finite dimensional control



Conclusions:

- Stantard numerical schemes have to be "tuned" to guarantee convergence in the nonlinear setting.
- Dissipation and two-grid filtering mechanisms help.
- Our analysis relies on Fourier transform. Much remains to be done to deal with more general modelas and non-uniform meshes.
- Similar pathologies and cures may arise also on control problems.
- The analysis developed here may also be relevant in other issues such as the transparent boundary conditions: What can they do if waves do not reach the boundary?
- ....
- ....
- Things might seem better in numerical experiments, but: WARNING: These effects are in!
- Be careful when transfering qualitative properties from the numerics to the PDE setting and viceversa.

Refs.

- E. Z. Propagation, observation, and control of waves approximated by finite difference methods. SIAM Review, 47 (2) (2005), 197-243.
- L. IGNAT & E. Z., Dispersive Properties of Numerical Schemes for Nonlinear Schrödinger Equations,Foundations of Computational Mathematics, Santander 2005, London Mathematical Society Lecture Notes, 331, L. M. Pardo et al. eds, Cambridge University Press, 2006, pp. 181-207.
- L. IGNAT and E. ZUAZUA, Convergence rates for dispersive approximation schemes to nonlinear Schrödinger equations, preprint, 2009.
- L. Ignat, M3AS, Vol. 17, No. 4 (2007) 567-591. (time discrete)

¡Thank you!

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