Dispersive schemes for linear and nonlinear Schrödinger equations

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Joint work with Enrique Zuazua

Outline

1. Introduction
2. Semidiscrete schemes
3. Fully discrete schemes
4. A splitting method
5. Conclusions

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Motivation

To build convergent numerical schemes for nonlinear PDE.

Example: Schrödinger equation

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

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

Key point: To handle nonlinearities one needs to use hidden properties of the underlying linear differential operators (Kato, Strichartz, Ginibre, Velo, Cazenave, Weissler, Saut, Bourgain, Kenig, Ponce, Saut, Vega, Burq, Gérard, Tzvetkov, ...)

This has been done successfully for the PDE models.

Nonlinear problems

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

$$u_t(t) = Au(t) + f(u(t)),\ t > 0,\ u(0) = u_0.$$

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

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

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

But, often in applications, the property that $f : H \to H$ is locally Lipshitz 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 $e^{At} \in X$, then look for solutions of the nonlinear problem in

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

One then needs to investigate whether

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

is locally Lipschitz. This require extra work: We need to check the behavior of f in the space X. But in the class of functions to be tested is restricted to those belonging to X.

Typically in applications $X = L^q(0,T;L^r(\Omega))$. 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!

Linear Schrödinger Equation

$$\begin{cases} iu_t + \Delta u = 0,\ x \in \mathbb{R}^d,\ t \neq 0, \\ u(0,x) = \varphi(x),\ x \in \mathbb{R}^d, \end{cases}$$

Conservation of the L^2-norm

$$\|S(t)\varphi\|_{L^2(\mathbb{R}^d)} = \|\varphi\|_{L^2(\mathbb{R}^d)}$$

Dispersive estimate

$$|S(t)\varphi(x)| \leq \frac{1}{(4\pi|t|)^{d/2}} \|\varphi\|_{L^1(\mathbb{R}^d)}$$

Space time estimates

The admissible pairs

$$\frac{2}{q} = d\left(\frac{1}{2} - \frac{1}{r}\right)$$

Strichartz estimates for admissible pairs (q, r)

$$\|S(\cdot)\varphi\|_{L^q(\mathbb{R},\, L^r(\mathbb{R}^d))} \leq C(q,r)\|\varphi\|_{L^2(\mathbb{R}^d)}$$

Local Smoothing effect

$$\sup_{x_0, R} \frac{1}{R} \int_{B(x_0,R)} \int_{-\infty}^{\infty} |(-\Delta)^{1/4} e^{it\Delta}\varphi|^2 dt dx \leq C\|\varphi\|^2_{L^2(\mathbb{R}^d)}$$

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Nonlinear Schrödinger Equation

$$\begin{cases} iu_t + \Delta u = |u|^p u, \, x \in \mathbb{R}^d, \, t \neq 0 \\ u(0,x) = \varphi(x), \, x \in \mathbb{R}^d \end{cases}$$

For initial data in $L^2(\mathbb{R}^d)$, Tsutsumi '87 proved the global existence and uniqueness for $p < 4/d$

$$u \in C(\mathbb{R}, \, L^2(\mathbb{R}^d)) \cap L^q_{loc}(\mathbb{R}, \, L^r(\mathbb{R}^d))$$

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

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A first numerical scheme for NSE

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = |u^h|^2 u^h, \quad t \neq 0, \\ \\ u^h(0) = \varphi^h. \end{cases}$$

Questions

- Does u^h converge to the solution of NSE?
- Is u^h uniformly bounded in $L^q_{loc}(\mathbb{R}, l^r(h\mathbb{Z}^d))$?
- Local Smoothing ?

Tools

- Semidiscrete Fourier transform

$$\widehat{v}(\xi) = (\mathcal{F}_h v)(\xi) = h^d \sum_{\mathbf{j}\in\mathbb{Z}^d} e^{-i\xi\cdot\mathbf{j}h} v_{\mathbf{j}},\ \xi \in [-\pi/h, \pi/h]^d$$

- Oscillatory integrals, Van der Corput Lemma, Fourier multipliers, Poisson Integrals
- Previous ideas of Keel & Tao '98, Kenig, Ponce & Vega '91, Christ & Kiselev '01, Constantin & Saut '89 ...

A conservative scheme for LSE

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

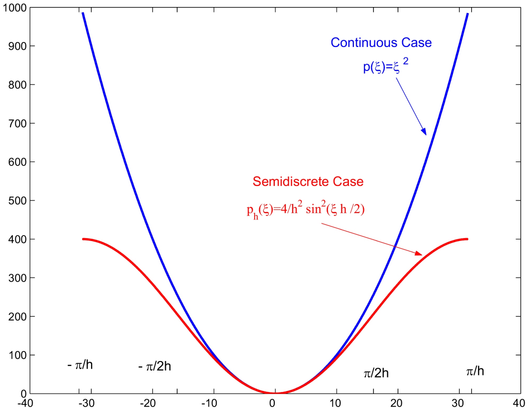
In the Fourier space the solution $\widehat{u}^h$ can be written as

$$\widehat{u}^h(t,\xi) = e^{itp_h(\xi)}\widehat{\varphi}^h(\xi),\ \xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]^d,$$

where

$$p_h(\xi) = \frac{4}{h^2}\sum_{k=1}^{d} \sin^2\left(\frac{\xi_k h}{2}\right).$$

The two symbols in dimension one



- Lack of uniform $l^1 \to l^\infty$: $\xi = \pm\pi/2h$
- Lack of uniform local smoothing effect: $\xi = \pm\pi/h$

Lemma

(Van der Corput) Suppose ψ is real-valued and smooth in (a,b), and that $|\psi^{(k)}(x)| \geq 1$ for all $x \in (a,b)$. Then

$$\left| \int_a^b e^{i\lambda\psi(x)} dx \right| \leq c_k \lambda^{-1/k}$$

In dimension one:

$$\frac{\|u^h(t)\|_{l^\infty(h\mathbb{Z})}}{\|u^h(0)\|_{l^1(h\mathbb{Z})}} \lesssim \frac{1}{t^{1/2}} + \frac{1}{(th)^{1/3}}.$$

These slight changes on the shape of the symbol are not an obstacle for the convergence of the numerical scheme in the $L^2(\mathbb{R})$ sense for LSE. But produce the lack of uniform (in h) dispersion of the numerical scheme and consequently, makes the scheme useless for nonlinear problems.

Theorem

Let $T > 0$, $r_0 \geq 1$ *and* $r > r_0$. *Then*

$$\sup_{h>0,\,\varphi\in l^r(h\mathbb{Z}^d)} \frac{\|S^h(\cdot)\varphi\|_{L^1((0,T),l^r(h\mathbb{Z}^d))}}{\|\varphi\|_{l^{r_0}(h\mathbb{Z}^d)}} = \infty.$$

Proof.

Wave packets concentrated at $(\pi/2h)^d$ $\square$

Filtering initial data

Initial data supported far from $(\pm\pi/2h)^d$

- $\|S^h(t)\varphi\|_{l^\infty(h\mathbb{Z}^d)} \lesssim \frac{1}{|t|^{d/2}}\|\varphi\|_{l^1(h\mathbb{Z}^d)}$
- Strichartz like estimates: $\|S^h(\cdot)\varphi\|_{L^q(\mathbb{R},l^r(h\mathbb{Z}^d))} \lesssim \|\varphi\|_{l^2(h\mathbb{Z}^d)}$

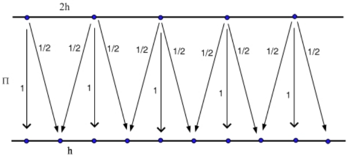
Initial data supported far from $(\pm\pi/h)^d$

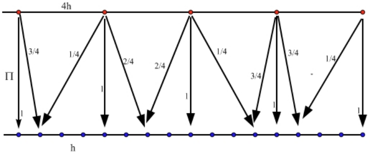
- Gain of 1/2 local space derivative

Two-grid method, Glowinski '90

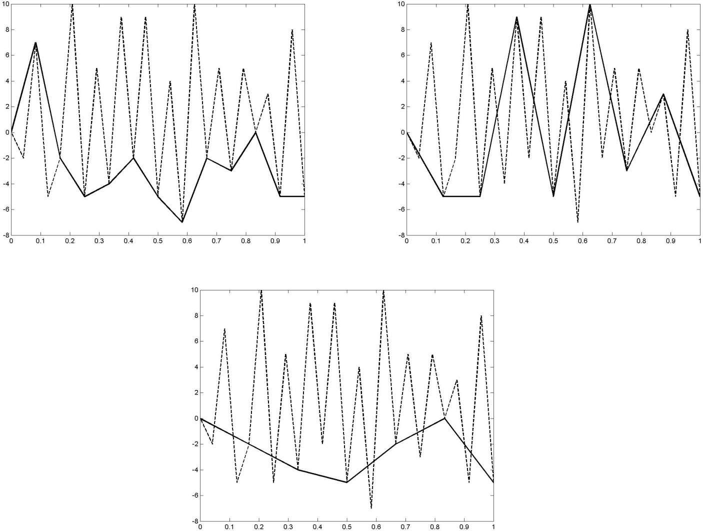
A TWO-GRID ALGORITHM= A CONSERVATIVE SCHEME

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





Various type of two-grid methods: 1/2, 1/3, 1/4



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

Expansion and restriction operators

I-multilinear interpolator on $4h\mathbb{Z}^d$

$\widetilde{\Pi} : l^2(4h\mathbb{Z}^d) \to l^2(h\mathbb{Z}^d)$ defined by $(\widetilde{\Pi} f)_{\mathbf{j}} = (If)_{\mathbf{j}}, \quad \mathbf{j} \in \mathbb{Z}^d$

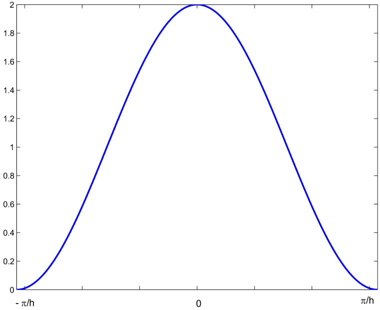
$\widetilde{\Pi}^* : l^2(h\mathbb{Z}^d) \to l^2(4h\mathbb{Z}^d)$: $(\widetilde{\Pi} f, g)_{l^2(h\mathbb{Z}^d)} = (f, \widetilde{\Pi}^* g)_{l^2(4h\mathbb{Z}^d)}$

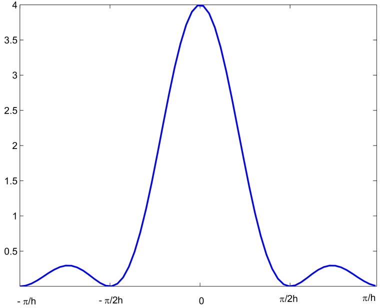
Explicit expressions

$$(\widetilde{\Pi} f)_{4j+r} = \frac{4-r}{4} f_{4j} + \frac{r}{4} f_{4j+4}, \; j \in \mathbb{Z}, \; r \in \{0, 1, 2, 3\}$$

$$(\widetilde{\Pi}^* g)_{4j} = \sum_{r=0}^{3} \frac{4-r}{4} g_{4j+r} + \frac{r}{4} g_{4j-4+r}, \; j \in \mathbb{Z}.$$

Fourier analysis





$$\widehat{\widetilde{\Pi}\psi}(\xi) = 2\widehat{\psi}(\xi)\cos^2\left(\frac{\xi h}{2}\right),\ \psi \in l^2(2h\mathbb{Z})$$

$$\widehat{\widetilde{\Pi}\psi}(\xi) = 4\widehat{\psi}(\xi)\cos^2(\xi h)\cos^2\left(\frac{\xi h}{2}\right),\ \psi \in l^2(4h\mathbb{Z}^d)$$

Key estimates

Dispersive estimate

$$\|e^{it\Delta_h}\widetilde{\Pi}\varphi\|_{l^\infty(h\mathbb{Z}^d)} \leq C(d,p)|t|^{-d/2}\|\widetilde{\Pi}\varphi\|_{l^1(h\mathbb{Z}^d)}$$

Proof: Careful application of Kenig, Ponce and Vega '91 results

Application to a nonlinear problem with $L^2(\mathbb{R}^d)$ initial data

$$\begin{cases} iu_t + \Delta u = |u|^p u,\ t > 0, \\ u(0,x) = \varphi(x),\ x \in \mathbb{R}^d, \end{cases}$$

An approximation

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = \widetilde{\Pi} f(\widetilde{\Pi}^* u^h),\ t \in \mathbb{R} \\ \\ u^h(0) = \widetilde{\Pi}\varphi^h, \end{cases} \tag{1}$$

where $f(u) = |u|^p u$

$$u^h \in G_h \to \widetilde{\Pi}^* u^h \in G_{4h} \to \widetilde{\Pi} f(\widetilde{\Pi}^* u^h) \in G_h$$

Key point

$$(\widetilde{\Pi} f(\widetilde{\Pi}^* u^h), u^h)_{l^2(h\mathbb{Z}^d)} = (f(\widetilde{\Pi}^* u^h), \widetilde{\Pi}^* u^h)_{l^2(4h\mathbb{Z}^d)} \in \mathbb{R}$$

Convergence of the method

Theorem

Let E be the piecewise constant interpolator. The sequence Eu^h satisfies

$$Eu^h \overset{\star}{\rightharpoonup} u \text{ in } L^\infty(\mathbb{R}, L^2(\mathbb{R}^d)),\ Eu^h \rightharpoonup u \text{ in } L^q_{loc}(\mathbb{R}, L^{p+2}(\mathbb{R}^d)),$$

$$Eu^h \to u \text{ in } L^2_{loc}(\mathbb{R}^{d+1}),\ E\widetilde{\Pi} f(\widetilde{\Pi}^* u^h) \rightharpoonup |u|^p u \text{ in } L^{q'}_{loc}(\mathbb{R}, L^{(p+2)'}(\mathbb{R}^d))$$

where u is the unique solution of NSE.

- Main difficulty - passing to the limit in the nonlinear term
- $\ddot\smile$ Local smoothing effect of the linear semigroup for two-grid data $\mapsto$ compactness ...

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Fully Discrete Schemes

Two level schemes satisfying stability and consistency:

$$U^{n+1} = A_\lambda U^n, n \geq 0$$

where $\lambda = k/h^2$ is keep constant

Two goals:

1. $l^1 - l^\infty$ decay of solutions
2. local smoothing effect

Fourier analysis: A_λ has a symbol $a_\lambda = m_\lambda \exp(i\psi_\lambda)$

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Fourier analysis: A_λ has a symbol $a_\lambda = m_\lambda \exp(i\psi_\lambda)$

Decay properties

Theorem

Let us assume that the symbol a_λ has the following property

$$m_\lambda(\xi_0) = 1 \quad \Rightarrow \quad |\psi''_\lambda(\xi_0)| > 0 \ \textit{ or } \ m''_\lambda(\xi_0) \neq 0.$$

Then there is a positive constant $C(\lambda)$ such that

$$\|S_\lambda(n)\varphi\|_{l^\infty(h\mathbb{Z})} \leq C(\lambda)(nk)^{-\frac{1}{2}}\|\varphi\|_{l^1(h\mathbb{Z})}$$

holds for all $n \neq 0$, $h, k > 0$.

Local smoothing effect

Theorem

There is a positive s and a constant $C(s,\lambda)$ such that

$$k\sum_{nk\leq 1}\left[h\sum_{|j|h\leq 1}|((-\Delta_h)^{s/2}U^n)_j|^2\right]\leq C(s,\lambda)\left[h\sum_{j\in\mathbb{Z}}|U_j^0|^2\right] \qquad (2)$$

holds for all $\varphi\in l^2(h\mathbb{Z})$ and for all $h>0$ if and only if the symbol a_λ satisfies

$$\xi_0\neq 0,\ \psi'_\lambda(\xi_0)=0 \quad\Rightarrow\quad m_\lambda(\xi_0)<1. \qquad (3)$$

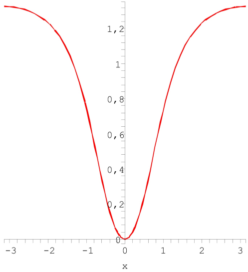
Moreover if (3) holds then $s=1/2$.

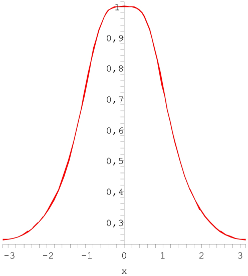
Backward Euler

$$i\frac{U_j^{n+1}-U_j^n}{k}+\frac{U_{j+1}^{n+1}-2U_j^{n+1}+U_{j-1}^{n+1}}{h^2}=0,\ n\geq 0,\ j\in\mathbb{Z},$$

$$a_\lambda(\xi)=\frac{1}{1-4i\lambda\sin^2\frac{\xi}{2}}=\frac{\exp(i\arctan(4\lambda\sin^2\frac{\xi}{2}))}{\left(1+16\lambda^2\sin^4\frac{\xi}{2}\right)^{1/2}}$$

The symbols ψ_1 and m_1



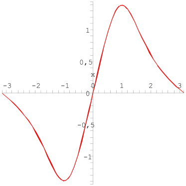


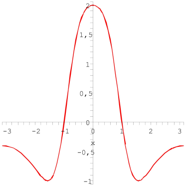
Crank-Nicolson scheme

$$i\frac{U_j^{n+1}-U_j^n}{k}+\frac{U_{j+1}^{n+1}-2U_j^{n+1}+U_{j-1}^{n+1}}{2h^2}+\frac{U_{j+1}^{n}-2U_j^{n}+U_{j-1}^{n}}{2h^2}=0$$

$$a_\lambda(\xi)=\frac{1+2i\lambda\sin^2\frac{\xi}{2}}{1-2i\lambda\sin^2\frac{\xi}{2}}=\exp\left(2i\arctan\left(2\lambda\sin^2\frac{\xi}{2}\right)\right)$$

The first two derivatives ψ_1' and ψ_1''





Crank-Nicolson scheme

For any $\lambda \in \mathbb{Q}$

- There is no two-grid algorithm involving the grids $ph\mathbb{Z}$ and $h\mathbb{Z}$ which would provide a $l^1 - l^\infty$ uniform decay
- The involved function ψ''_λ has roots on $[-\pi, \pi] \backslash \pi\mathbb{Q}$, thus cyclothomic polynomials ...

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A simple construction

Define the flow $S(t)$ of the linear Schrödinger equation

$$\begin{cases} iu_t + \Delta u = 0, & x \in \mathbb{R}^d,\ t \neq 0, \\ u(0,x) = \varphi(x), & x \in \mathbb{R}^d \end{cases}$$

and the flow $N(t)$ for the differential equation

$$\begin{cases} \dfrac{du}{dt} = i|u|^p u, & x \in \mathbb{R},\ t > 0, \\ u(x,0) = \varphi(x), & x \in \mathbb{R}. \end{cases}$$

$$Z(n\tau) := (S(\tau)N(\tau))^n \varphi,\ 0 \leq n\tau \leq T.$$

May we guarantee that Z belongs to auxiliary space $l^q(0,T;L^r(\mathbb{R}))$?

In general no! There exists $\varphi \in L^2(\mathbb{R})$ such that for any $r > 2$

$$Z(\tau) = S(\tau)N(\tau)\varphi \notin L^r(\mathbb{R}).$$

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A new construction

Remedy: consider discrete spaces instead of continuous one. Thus all the quantities make sense since $l^1(h\mathbb{Z}) \subset l^2(h\mathbb{Z}) \subset l^\infty(h\mathbb{Z})$.

New approximation:

$$Z^h(n\tau) = (S^h(\tau)N^h(\tau))^n\varphi^h,\ 0 \leq n\tau \leq T$$

where S^h is a fully discrete approximation of the LSE (Backward Euler) and N^h solves the discrete ODE:

$$\begin{cases} \dfrac{du_j^h}{dt} = i|u_j|^p u_j, & j \in \mathbb{Z}, t > 0, \\ u_j(0) = \varphi_j, & j \in \mathbb{Z}. \end{cases}$$

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How to prove the uniform boundedness in the space $l^q(0,T;\, l^r(h\mathbb{Z}))$?

Write in semigroup like formulation and use the qualitative properties of the approximation S^h:

$$Z^h(n\tau) = S^h(n\tau)N^h(\tau)\varphi^h + \sum_{k=1}^{n-1} S^h((n-k)\tau)(N^h(\tau)-I)Z^h(k\tau)$$

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Uniform boundedness

Theorem

Let $p < 4$, τ and h be such that τ/h^2 is keep constant. Also let S^h be an approximation of $S(\cdot)$ given by a consistent and L^2-stable numerical scheme that has an $l^1(h\mathbb{Z}) - l^\infty(h\mathbb{Z})$-decay as $t^{-1/2}$. The approximate solution Z^h satisfies

$$\|Z^h(\cdot\tau)\|_{l^\infty(\mathbb{Z};\, l^2(h\mathbb{Z}))} \leq \|\varphi^h\|_{l^2(h\mathbb{Z})}. \tag{4}$$

Moreover, for any $T > 0$ and (q, r) admissible-pair there exists a positive constant $C(T, r)$ such that

$$\|Z^h(\cdot\tau)\|_{l^q(|n|\tau\leq T;\, l^r(h\mathbb{Z}))} \leq C(T, r)\|\varphi^h\|_{l^2(h\mathbb{Z})}. \tag{5}$$

Sketch of the proof

Choose $C > 0$ such that

$$\Lambda = \left\{ N \in \mathbb{Z}, N \geq 0, \left(\tau \sum_{k=0}^{N} \|Z^h(k\tau)\|_{l^r(h\mathbb{Z})}^q \right)^{1/q} \leq C\|\varphi^h\|_{l^2(h\mathbb{Z})} \right\}.$$

is no empty: $0 \in \Lambda$

Prove that its maximal element N^* is either infinity or

$$N^*\tau \geq C(\|\varphi^h\|_{l^2(h\mathbb{Z})})$$

Sketch of the proof

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Prove that its maximal element N^* is either infinity or

$$N^* \tau \geq C(\|\varphi^h\|_{l^2(h\mathbb{Z})})$$

Convergence

Theorem

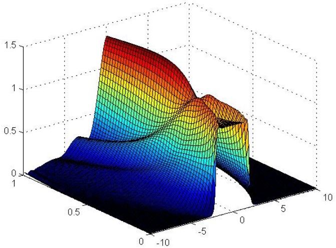
Let $\varphi \in L^2(\mathbb{R})$ and φ^h such that $\varphi^h \to \varphi$ in $L^2(\mathbb{R})$. Then there exists $T = T(\|\varphi\|_{L^2(\mathbb{R})})$ such that for any $\epsilon > 0$ there exists $h_0 = h_0(\epsilon)$ such that

$$\|Z^h - \underline{u}_h\|_{l^\infty(|n|\tau \le T;\, l^2(h\mathbb{Z}))} + \|Z^h - \underline{u}_h\|_{l^q(|n|\tau \le T;\, l^r(h\mathbb{Z}))} \le \epsilon \tag{6}$$

holds for all $h \le h_0$.

An experiment

We work with initial data the $\varphi = \chi_{(-2,2)}$ and the computational domain $(-10, 10)$.



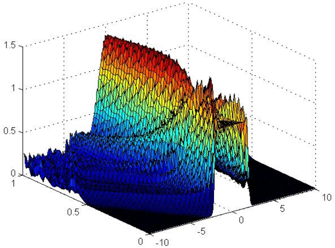


Figure: Solutions obtained with backward Euler and Crank-Nicolson scheme, $h = 0.1$, $\tau = 0.01$

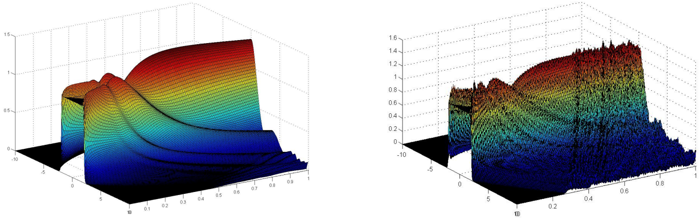


Figure: Solutions obtained with backward Euler and Crank-Nicolson scheme, $h = 0.05$, $\tau = 0.0025$

Outline

1. Introduction
2. Semidiscrete schemes
3. Fully discrete schemes
4. A splitting method
5. Conclusions

Conclusions

- Fourier filtering (and some other variants like numerical viscosity, and two-grid filtering, ...) allow building numerical schemes for an efficient approximation of linear and nonlinear Schrödinger equations.
- these new schemes allow capturing the right dispersion properties of the continuous models and consequently provide convergent approximations for nonlinear equations too.
- the computational cost for the nonlinear problem is the same as for the linear one
- MUCH REMAINS TO BE DONE
  BOUNDARY-VALUE PROBLEMS, NONREGULAR MESHES, OTHER PDE'S,...

References

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L.I., *Fully discrete schemes for the Schrödinger equation: Dispersive properties*, Mathematical Models and Methods in Applied Sciences, Vol. 17, No. 4 (2007) 567-591.

See also
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THANKS!