Schrödinger Equations, Numerical Approximation Schemes and Dispersive Properties

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The Linear Schrödinger Equation

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

Dispersive Properties

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

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

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

- 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 non only relevant for a better understanding of the dynamics of the linear system but also to derive well-posedness results for nonlinear Schrödinger equation (NSE).

Preliminaries

- For $1 \leq p < \infty$ we define the spaces $l_h^p(\mathbf{Z})$ as
$$l_h^p(\mathbf{Z}) = \{(\varphi_j)_{j\in\mathbf{Z}} \in \mathbf{C}^{\mathbf{Z}} : h \sum_{j\in\mathbf{Z}} |\varphi_j|^p < \infty\}.$$

- If $p = \infty$ we set
$$l_h^\infty(\mathbf{Z}) = \{(\varphi_j)_{j\in\mathbf{Z}} : \sup_{j\in\mathbf{Z}} |\varphi_j| < \infty\},$$

- The discrete convolution $((a \star b)_j)_{j\in\mathbf{Z}}$ of two sequences $(a_j)_{j\in\mathbf{Z}}$ and $(b_j)_{j\in\mathbf{Z}}$ is defined by
$$(a \star b)_j = h \sum_{n\in\mathbf{Z}} a_{j-n} b_n = h \sum_{n\in\mathbf{Z}} a_n b_{j-n}$$

- If $v \in l_h^2$, then the semidiscrete Fourier transform

$$\hat{v}(\xi) = h \sum_{j \in \mathbf{Z}} e^{-ijh\xi} v_j, \qquad \xi \in [-\frac{\pi}{h}, \frac{\pi}{h}]$$

  belongs to L_h^2, and v can be recovered from $\hat{v}$ by the **inverse semidiscrete Fourier transform**

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

  The l_h^2-norm of v and the L_h^2-norm of $\hat{v}$ are related by **Parseval's equality**,

$$\|\hat{v}\|_{L_h^2} = \sqrt{2\pi} \|v\|_{l_h^2}.$$

Consider the finite difference approximation

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

Here u^h stands for the infinite vector unknown $\{u_j^h\}_{j\in\mathbf{Z}}$,, $u_j(t)$ being the approximation of the solution at the node $x_j = jh$, and Δ_h being the classical second order finite difference approximation of ∂_x^2:

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

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

The same convergence result holds for semilinear equations

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

provided that 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 the NSE is also well-posed for some nonlinearities that grow superlinealy at infinity,

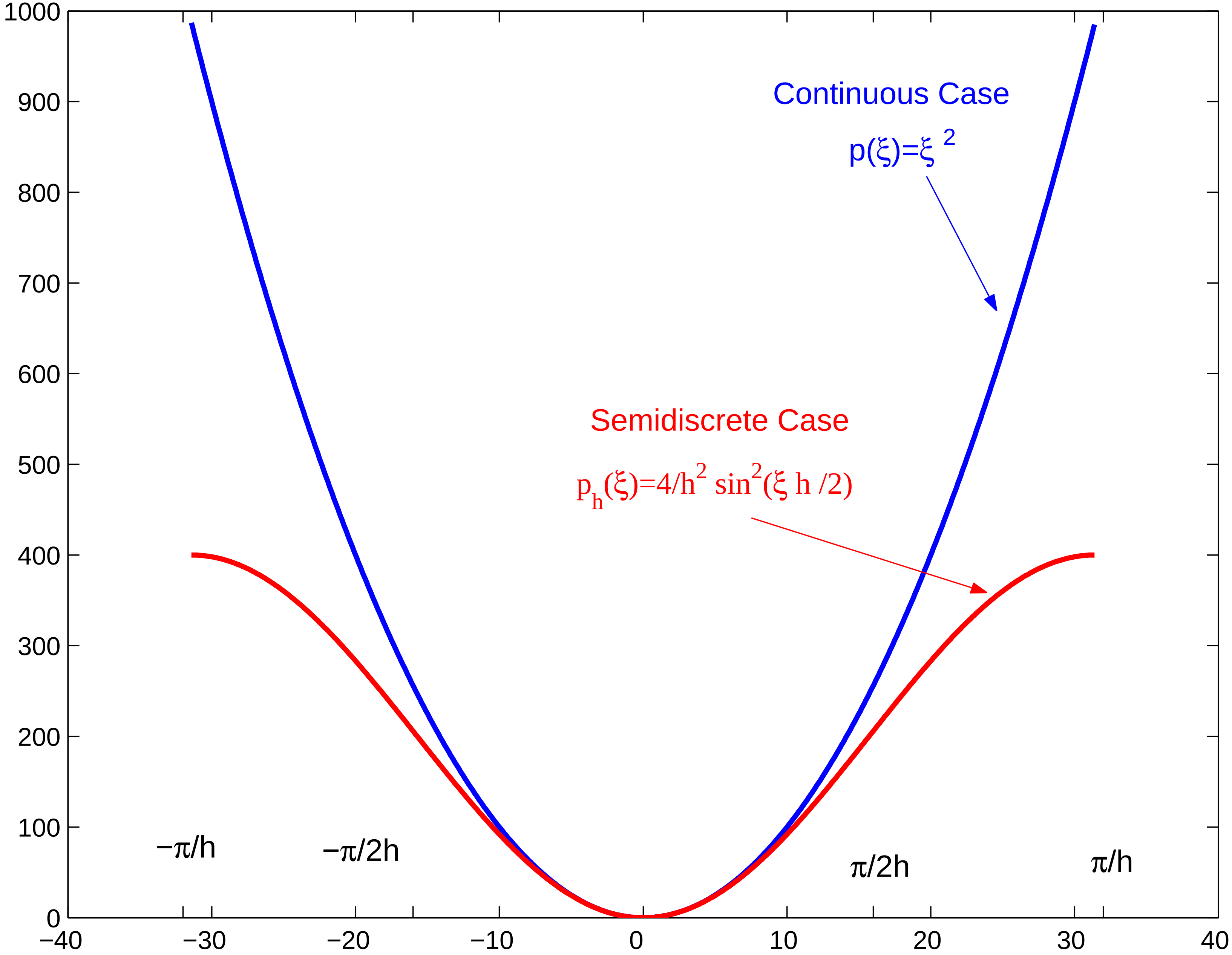
But this well-posedness result may not be proved simply as a consequence of the L^2-conservation property. The dispersive properties of the LSE play a key role.

Accordingly, one may not expect to prove convergence of the numerical schemes without similar dispersive estimates, that should be uniform on the mesh-size parameter $h \to 0$.

There are “slight” but important difference between the symbols of the operators $-\Delta$ and $-\Delta_h$:

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

For a fixed frequency ξ, obviously, $p_h(\xi) \to p(\xi)$, as $h \to 0$ but this is far from being sufficient for our 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

1. $p(\xi)$ is a convex function;

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

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

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

The explicit solution of (2) is

$$u_j^h(t) = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} \exp\left(-i\frac{4t}{h^2}\sin^2(\frac{\xi h}{2})\right) \hat{\varphi}^h(\xi)e^{ijh\xi}d\xi. \qquad (4)$$

By a simple change o variables

$$u_j^h(t) = u_j^1(\frac{t}{h^2})$$

$$\frac{\|\exp(it\Delta_h\varphi^h)\|_{l_h^p(\mathbf{Z})}}{\|\varphi^h\|_{l_h^{p'}(\mathbf{Z})}} = h^{\frac{1}{p}-\frac{1}{p'}}\frac{\|\exp(i\frac{t}{h^2}\Delta_1\varphi^1)\|_{l_1^p(\mathbf{Z})}}{\|\varphi^1\|_{l_1^{p'}(\mathbf{Z})}}$$

Fundamental Solutions of Equation (2) are given by

$$(K_t^h)_\nu = e^{-i\frac{t}{h^2}} i^\nu J_\nu(\frac{t}{h^2})$$

where $J_\nu(x)$ is the Bessel Function.

Using estimates for Bessel Function (J.A. Barcelo, A.Cordoba) we can obtain :

Theorem 1. *Let $p \geq 4$. Then, for all positive t,*

$$\sup_{h>0, \varphi^h \in l_h^{p'}(\mathbf{Z})} \frac{\| \exp(it\Delta_h \varphi^h) \|_{l_h^p(\mathbf{Z})}}{\|\varphi^h\|_{l_h^{p'}(\mathbf{Z})}} = \infty$$

Filtering of the frequencies close to $\pm\frac{\pi}{2h}$ suffices to recover the right decay properties :

Theorem 2. *Let* $\delta > 0$*. Then there is a constant* $c(\delta)$ *such that*

$$\|u^h(t)\|_{l_h^\infty(\mathbf{Z})} \leq \frac{c(\delta)}{\sqrt{t}} \|\varphi^h\|_{l_h^1(\mathbf{Z})}$$

for all $\varphi \in l_h^1(\mathbf{Z})$ with supp$\overset{\sqcap}{\varphi}^h \cap [\pm\frac{\pi}{2h} - \delta, \pm\frac{\pi}{2h} + \delta] = \emptyset$, uniformly in $h > 0$.

Concerning the local smoothing we have :

Theorem 3. *Let* $\delta > 0$, $\psi \in \mathcal{D}(\mathbf{R})$ *and* E^h *be a piecewise linear interpolant. Then there is constant* $C(\delta, \psi)$ *such that*

$$\|\psi E^h u^h\|_{L^2(\mathbf{R}, H^{1/2}(\mathbf{R}))} \leq c(\delta, \psi) \|\varphi^h\|_{l^2_h(\mathbf{Z})}$$

for all $\varphi^h \in l^2_h(\mathbf{Z})$ *with* $\mathrm{supp} \overset{\sqcap}{\varphi}^h \subset \left[-\frac{\pi-\delta}{h}, \frac{\pi-\delta}{h}\right]$, *uniformly in* $h > 0$.

But Fourier filtering is of little use in nonlinear problems.

As an alternative remedy we propose adding some artificial numerical viscosity term. This should be done so that:

- The new scheme should be convergent for LSE;

- It should posses the dispersivity properties of the LSE

The second property , the much more subtle one, should be achievable if the numerical viscosity term is efficient enough to damp out the high frequencies that are responsible of the lack of dispersivity of the simplest conservative scheme.

Consider

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

where $a(h) > 0$ is such that

$$a(h) \to 0$$

as $h \to 0$.

This scheme generates a semigroup $S_+^h(t)$, for $t > 0$. Similarly one may define $S_-^h(t)$, for $t < 0$.

The semigroup is dissipative in L^2. Thus the L^2-stability and convergence is guaranteed.

Discrete Heat Equation

$$\begin{cases} \dfrac{du_j^h}{dt} = \dfrac{u_{j+1}^h - 2u_j^h + u_{j-1}^h}{h^2}, & t > 0\,, j \in \mathbf{Z} \\ u_j^h(0) = \varphi_j^h, & j \in \mathbf{Z}, \end{cases} \tag{5}$$

Decay Properties

Theorem 4. *Let $1 \le q \le p \le \infty$. Then there exists a positive constant $c(p,q)$ such that*

$$\|u^h(t)\|_{l_h^p(\mathbf{Z})} \le c(p,q) t^{-\frac{1}{2}(\frac{1}{q}-\frac{1}{p})} \|\varphi^h\|_{l_h^q(\mathbf{Z})}. \tag{6}$$

Exact solution

$$u^h(t) = H_t^h \star \varphi^h$$

where

$$(H_t^h)_j = \frac{1}{2\pi} \int_{-\frac{\pi}{h}}^{\frac{\pi}{h}} e^{-\frac{4t}{h^2}\sin^2(\frac{\theta h}{2})} e^{ijh\theta} d\theta. \tag{7}$$

Theorem 5. *If $1 \leq p \leq \infty$, then there is a positive constant $C(p)$ independent of h, such that*

$$\|H_t^h\|_{l_h^p(\mathbf{Z})} \leq C(p) t^{-\frac{1}{2}(1-\frac{1}{p})}, \ \forall \ t > 0. \tag{8}$$

Proof

$$p = \infty$$

$$p = 1$$

Lemma 1. *(Carlson - Beurling Inequality) Assume that* $a \in L^2(\mathbf{R})$*,* $a' \in L^2(\mathbf{R})$*. Then* $\widehat{a} \in L^1(\mathbf{R})$ *and*

$$\|\widehat{a}\|_{L^1(\mathbf{R})} \leq (2\|a\|_{L^2(\mathbf{R})}\|a'\|_{L^2(\mathbf{R})})^{\frac{1}{2}} \tag{9}$$

Back to LSH

The main dispersive properties are as follows :

Theorem 6. *(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

$$\|S^h_\pm(t)\varphi^h\|_{l^p_h(\mathbf{Z})} \leq c(p)(|t|^{-\alpha(1-\frac{2}{p})} + |t|^{-\frac{1}{2}(1-\frac{2}{p})})\|\varphi^h\|_{l^{p'}_h(\mathbf{Z})} \qquad (10)$$

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

Sketch of the Proof

$$S_+^h(t)\varphi^h = K_t^h \star \varphi^h$$

$$\widehat{K_t^h} = e^{-itp_h(\xi)} e^{-ta(h)p_h(\xi)}$$

It is sufficient to prove

$$\|K_t^h\|_{l^\infty(\mathbf{Z})} \leq \frac{1}{t^\alpha} + \frac{1}{t^{1/2}}$$

$$
\begin{cases}
K_t^h = K_{t,low}^h + K_{t,high}^h \\
\widehat{K}^{h}_{t,low} = \widehat{K}^{h}_{t}\,\chi_{(-\pi/4h,\pi/4h)}
\end{cases}
$$

- $\|K_{t,high}^h\|_{l^\infty(\mathbf{Z})} \leq \frac{1}{t^\alpha}$ - brute force

- $K_{t,low}^h = H_{a(h)t}^h \star K_t^{1,h}$ where $\widehat{K}_t^{1,h} = e^{-itp_h(\xi)}\chi_{(-\pi/4h,\pi/4h)}$

Theorem 7. *(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*

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

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

Putting these price together we conclude that the evolution operator

$$\mathcal{T}^h(t) = \begin{cases} S_+^h(t) & t > 0 \\ I & t = 0 \\ S_-^h(t) & t < 0, \end{cases}$$

which provides a convergent approximation of the LSE in the L^2-sense also satisfies :

Theorem 8. *For $r \geq 2$ and $\alpha \in (1/2, 1]$, there exists a constant $c(r)$ such that*

$$\|\mathcal{T}^h(t)^* \mathcal{T}^h(s) f^h\|_{l_h^r(\mathbf{Z})} \leq c(r)|t-s|^{-\alpha(1-\frac{2}{r})} \|f^h\|_{l_h^{r'}(\mathbf{Z})} \tag{11}$$

holds for all reals numbers $t \neq s$ which satisfy $|t-s| \leq 1$.

Let I be an interval of $\mathbf{R}$ with $|I| \leq 1$. The following properties hold :

1. $t \to \mathcal{T}^h(t)\varphi^h$ maps continuously $l^2_h(\mathbf{Z})$ to $L^q(I, l^r_h(\mathbf{Z})) \cap C(I, l^2_h(\mathbf{Z}))$ for every α-admissible pair (q, r).

2. A similar result holds for the non-homogenous equation.

The pair (q, r) is said to be α-admissible if

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

with $2 \leq r \leq \infty$.

For the LSE, the admissible pairs are those that correspond to $\alpha = 1/2$.

Note that, for the numerical scheme under consideration, we can not take $\alpha = 1/2$. Otherwise, the scheme would not converge to the LSE but rather to a viscous LSE.

But we can take $\alpha = \alpha(h)$ in such way that

$$\alpha(h) \to \frac{1}{2} \text{ as } h \to 0.$$

NUMERICAL APPROXIMATION OF THE NSE

Consider now :

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

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

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

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

Let us recall the following classical result:

Theorem 9. *(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 $C(\mathbf{R}, L^2(\mathbf{R})) \cap L^q_{loc}(L^{p+2}(\mathbf{R}))$ 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

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

with $0 \leq p < 4$ and

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

such that

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

as $h \downarrow 0$.

Theorem 10. *(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 $\varphi^h \in l^2_h(\mathbf{Z})$, *there exists a unique global solution*

$$u^h \in C([0,\infty), l^2_h(\mathbf{Z})) \cap L^q_{loc}([0,\infty); l^{p+2}_h(\mathbf{Z}))$$

of the problem (12) which satisfies the following estimates

$$\|u^h\|_{L^\infty(\mathbf{R}, l^2_h(\mathbf{Z}))} \leq \|\varphi\|_{l^2_h(\mathbf{Z})} \tag{13}$$

and

$$\|u^h\|_{L^{q(h)}(I, l^{p+2}_h(\mathbf{Z}))} \leq c(I)\|\varphi\|_{l^2_h(\mathbf{Z})} \tag{14}$$

where the above constants are independent of h.

Theorem 11. *(Convergence as $h \to 0$) The sequence Eu^h satisfies*

$$Eu^h \overset{\star}{\rightharpoonup} u \text{ in } \; L^\infty([0,\infty), L^2(\mathbf{R})), \tag{15}$$

$$Eu^h \rightharpoonup u \text{ in } \; L^s_{loc}([0,\infty), L^{p+2}(\mathbf{R})), \forall\, s < q, \tag{16}$$

$$Eu^h \to u \text{ in } \; L^2_{loc}([0,\infty) \times \mathbf{R}), \tag{17}$$

$$|Eu^h|^p |Eu^h| \to |u|^p u \text{ in } \; L^{q'}_{loc}([0,\infty), L^{(p+2)'}(\mathbf{R})) \tag{18}$$

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

Conclusions

- The method of numerical viscosity also works in order to approximate the N- dimensional NLS Cauchy problem

- The same methods seem to work in the case of periodic LSE

- Much remains to be done
  - Multigrid Methods
  - KDV,Waves