1

Dispersive Properties of Numerical Schemes for Nonlinear Schrödinger Equations

Liviu I. Ignat, Enrique Zuazua

Departamento de Matemáticas, Facultad de Ciencias,

Universidad Autónoma de Madrid, 28049 Madrid, Spain

liviu.ignat@uam.es, enrique.zuazua@uam.es

Abstract

In this article we report on recent work on building numerical approximation schemes for nonlinear Schrödinger equations. We first consider finite-difference space semi-discretizations and show that the standard conservative scheme does not reproduce at the discrete level the dispersion properties of the continuous Schrödinger equation. This is due to high frequency numerical spurious solutions. In order to damp out or filter these high-frequencies and to reflect the properties of the continuous problem we propose two remedies. First, adding a suitable extra numerical viscosity term at a convenient scale, and, second, a two-grid filter of the initial datum with meshes of ratio 1/4. We prove that these alternate schemes preserve the dispersion properties of the continuous model. We also present some applications to the numerical approximation of nonlinear Schrödinger equations with initial data in L^2. Despite the fact that classical energy methods fail, using these dispersion properties, the numerical solutions of the semi-discrete nonlinear problems are proved to converge to the solution of the nonlinear Schrödinger equation. We also discuss some open problems and some possible directions of future research.

1.1 Introduction

Let us consider the $1-d$ linear Schrödinger Equation (LSE) on the whole line

$$\begin{cases} iu_t + u_{xx} = 0, \ x \in \mathbf{R}, \ t \neq 0, \\ u(0,x) = \varphi(x), \ x \in \mathbf{R}. \end{cases} \tag{1.1}$$

The solution is given by $u(t) = S(t)\varphi$, where $S(t) = e^{it\Delta}$ is the free Schrödinger operator which defines a unitary transformation group in $L^2(\mathbf{R})$. The linear semigroup has two important properties, the conservation of the L^2-norm

$$\|u(t)\|_{L^2(\mathbf{R})} = \|\varphi\|_{L^2(\mathbf{R})} \tag{1.2}$$

and a dispersive estimate :

$$|u(t,x)| \leq \frac{1}{\sqrt{4\pi|t|}}\|\varphi\|_{L^1(\mathbf{R})}. \tag{1.3}$$

By classical arguments in the theory of dispersive equations the above estimates imply more general space-time estimates for the linear semigroup which allow proving the well-posedness of a wide class of nonlinear Schrödinger equations (cf. Strichartz (1977), Tsutsumi (1987), Cazenave (2003)).

In this paper we present some recent results on the qualitative properties of some numerical approximation schemes for the linear Schrödinger equation and its consequences in the context of nonlinear problems.

More precisely, we analyze whether these numerical approximation schemes have the same dispersive properties, uniformly with respect to the mesh-size h, as in the case of the continuous Schrödinger equation (1.1). In particular we analyze whether the decay rate (1.3) holds for the solutions of the numerical scheme, uniformly in h. The study of these dispersion properties of the numerical scheme in the linear framework is relevant also for proving their convergence in the nonlinear context. Indeed, since the proof of the well-posedness of the nonlinear Schrödinger equations in the continuous framework requires a delicate use of the dispersion properties, the proof of the convergence of the numerical scheme in the nonlinear context is hopeless if these dispersion properties are not verified at the numerical level.

To better illustrate the problems we shall address, let us first consider the conservative semi-discrete numerical scheme

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = 0,\ t \neq 0, \\ \\ u^h(0) = \varphi^h. \end{cases} \tag{1.4}$$

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

$$(\Delta_h u^h)_j = \frac{u^h_{j+1} - 2u^h_j + u^h_{j-1}}{h^2}.$$

This scheme satisfies the classical properties of consistency and stability which imply L^2-convergence. In fact stability holds because of the conservation of the discrete L^2-norm under the flow (1.4):

$$\frac{d}{dt}\left(h \sum_{j\in\mathbf{Z}} |u^h_j(t)|^2 \right) = 0. \tag{1.5}$$

The same convergence results hold for semilinear equations (NSE):

$$iu_t + u_{xx} = f(u) \tag{1.6}$$

provided that the nonlinearity f is globally Lipschitz continuous. But, it is by now well known (cf. Tsutsumi (1987), Cazenave (2003)) that the NSE is also well-posed for some nonlinearities that superlinearly grow at infinity. This well-posedness result cannot be proved simply as a consequence of the L^2 conservation property and the dispersive properties of the LSE play a key role.

Accordingly, one may not expect to prove convergence of the numerical scheme in this class of nonlinearities without similar dispersive estimates that should be uniform in the mesh-size parameter $h \to 0$. In particular, a discrete version of (1.3) is required to hold, uniformly in h. This difficulty may be avoided considering more smooth initial data φ, say, in $H^1(\mathbf{R})$, a space in which the Schrödinger equation generates a group of isometries and the nonlinearity is locally Lipschitz. But here, in order to compare the dynamics of the continuous and semi-discrete systems we focus on the $L^2(\mathbf{R})$-case, which is a natural class in which to solve the nonlinear Schrödinger equation.

In this article we first prove that the conservative scheme (1.4) fails to have uniform dispersive properties. We then introduce two numerical schemes for which the estimates are uniform. The first one uses an artificial numerical viscosity term and the second one involves a two-grid algorithm to precondition the initial data. Both approximation schemes of the linear semigroup converge and have uniform dispersion properties. This allows us to build two convergent numerical schemes for the NSE in the class of $L^2(\mathbf{R})$ initial data.

1.2 Notation and Preliminaries

In this section we introduce some notation that will be used in what follows: discrete l^p spaces, semidiscrete Fourier transform, discrete fractional differentiation, as well as the standard Strichartz estimates for the continuous equations.

The spaces $l^p(h\mathbf{Z})$, $1 \leq p < \infty$, consist of all complex-valued sequences $\{c_k\}_{k\in\mathbf{Z}}$ with

$$\|\{c_k\}\|_{l^p(h\mathbf{Z})} = \left(h \sum_{k\in\mathbf{Z}} |c_k|^p \right)^{1/p} < \infty.$$

In contrast to the continuous case, these spaces are nested:

$$l^1(h\mathbf{Z}) \subseteq l^2(h\mathbf{Z}) \subseteq l^\infty(h\mathbf{Z}).$$

The semidiscrete Fourier transform is a natural tool for the analysis of numerical methods for partial differential equations, where we are always concerned with functions defined on discrete grids. For any $u \in l^1(h\mathbf{Z})$, the semidiscrete Fourier transform of u at the scale h is the function $\hat{u}$ defined by

$$\hat{u}(\xi) = (\mathcal{F}_h v)(\xi) = h \sum_{j\in\mathbf{Z}} e^{-ijh\xi} u_j.$$

A priori, this sum defines a function $\hat{u}$ for all $\xi \in \mathbf{R}$. We remark that any wave number ξ is indistinguishable on the grid from all other wave numbers $\xi + 2\pi m/h$, where m is an integer, a phenomenon called aliasing. Thus, it is sufficient to consider the restriction of $\hat{u}$ to wave numbers in the range $[-\pi/h, \pi/h]$. Also u can be recovered from $\hat{u}$ by the inverse semidiscrete Fourier transform

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

We will also make use of a discrete version of fractional differentiation. For $\varphi \in l^2(h\mathbf{Z})$ and $0 \leq s < 1$ we define

$$(D^s \varphi)_j = \int_{-\pi/h}^{\pi/h} |\xi|^s \hat{\varphi}(\xi) e^{ijh\xi} d\xi.$$

Now, we make precise the classical dispersive estimates for the linear continuous Schrödinger semigroup $S(t)$. The energy and decay estimates (1.2) and (1.3) lead, by interpolation (cf. Bergh & Löfström (1976)), to the following $L^{p'} - L^p$ decay estimate:

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

for all $p \geq 2$ and $t \neq 0$. More refined space-time estimates known as the *Strichartz inequalities* (cf. Strichartz (1977), Ginibre & Velo (1992), Kell & Tao (1998)) show that, in addition to the decay of the solution as $t \to \infty$, a gain of spatial integrability occurs for $t > 0$. Namely

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

for suitable values of q and r, the so-called 1/2-admissible pairs. We recall that an α-admissible pair (q,r) satisfies

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

Also a local gain of 1/2 space derivative occurs in $L^2_{x,t}$ (cf. Constantin & Saut (1988), Kenig, Ponce & Vega (1991)):

$$\sup_{x_0,R} \frac{1}{R} \int_{B(x_0,R)} \int_{-\infty}^{\infty} |D_x^{1/2} e^{it\Delta} u_0|^2 dt dx \leq C\|u_0\|^2_{L^2(\mathbf{R})}.$$

1.3 Lack of Dispersion of the Conservative Semi-Discrete Scheme

Using the discrete Fourier transform, we remark that there are *slight* (see Fig. 1.1) but important differences between the symbols of the operators $-\Delta$ and $-\Delta_h$: $p(\xi) = \xi^2$, $\xi \in \mathbf{R}$ for $-\Delta$ and $p_h(\xi) = 4/h^2 \sin^2(\xi h/2)$, $\xi \in [\pi/h, \pi/h]$ for $-\Delta_h$. The symbol $p_h(\xi)$ changes convexity at the points $\xi = \pm\pi/2h$ and has critical points also at $\xi = \pm\pi/h$, two properties that the continuous symbol does not fulfil. As we will see, these pathologies affect the dispersive properties of the semi-discrete scheme.

Firstly we remark that $e^{it\Delta_h} = e^{it\Delta_1/h^2}$. Thus, by scaling, it is sufficient to consider the case $h = 1$ and the large time behavior of solutions for this mesh-size.

A useful tool to study the decay properties of solutions to dispersive equations is the classical Van der Corput lemma. Essentially it says that

$$\left|\int_a^b e^{it\psi(\xi)} d\xi\right| \lesssim t^{-1/k}$$

provided that ψ is real valued and smooth in (a,b) satisfying $|\partial^k\psi(x)| \geq 1$ for all $x \in (a,b)$. In the continuous case, i.e., with $\psi(\xi) = \xi^2$, using that the second derivative of the symbol is identically two ($\psi''(\xi) = 2$), one easily obtains (1.3). However, in the semi-discrete case the symbol

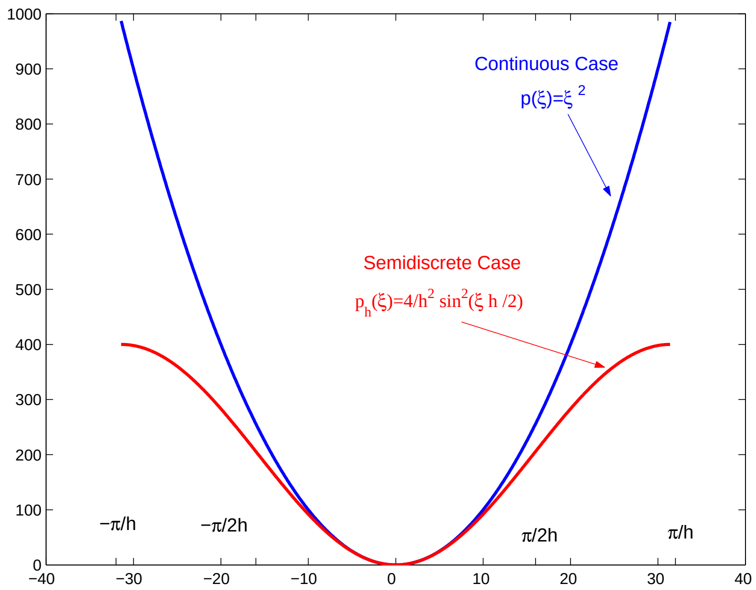

Fig. 1.1. The two symbols

of the semidiscrete approximation $p_1(\xi)$ satisfies

$$|\partial^2 p_1(\xi)| + |\partial^3 p_1(\xi)| \geq c$$

for some positive constant c, a property that the second derivative does not satisfy. This implies that for any t

$$\|u^1(t)\|_{l^\infty(\mathbf{Z})} \lesssim \left(\frac{1}{t^{1/2}} + \frac{1}{t^{1/3}}\right) \|u^1(0)\|_{l^1(\mathbf{Z})}. \tag{1.7}$$

This estimates was obtained in Stefanov & Kevrekidis (2005) for the semi-discrete Schrödinger equation in the lattice $\mathbf{Z}$. But here, we are interested on the behavior of the system as the mesh-size h tends to zero.

The decay estimate (1.7) contains two terms. The first one $t^{-1/2}$, is of the order of that of the continuous Schrödinger equation. The second term $t^{-1/3}$ is due to the discretization scheme and, more precisely, to the behavior of the semi-discrete symbol at the frequencies $\pm\pi/2$.
A scaling argument implies that

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

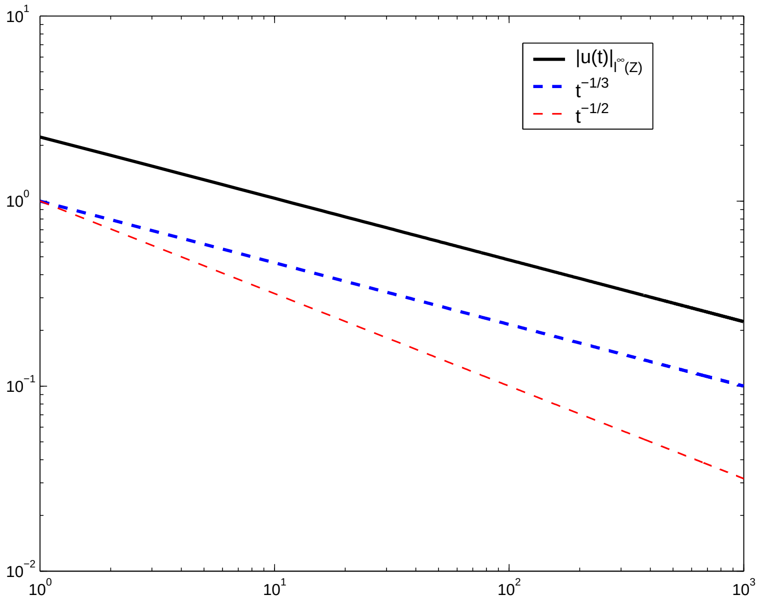

Fig. 1.2. Log-log plot of the time evolution of the l^∞ norm of u^1 with initial datum δ_0.

an estimate which fails to be uniform with respect to the mesh size h.

As we have seen, the $l^\infty(\mathbf{Z})$ norm of the discrete solution $u^1(t)$ behaves as $t^{-1/3}$ as $t \to \infty$. This is illustrated in Fig. 1.2 by choosing the discrete Dirac delta δ_0 as initial datum such that $u(0)_j = \delta_{0j}$ where δ is the Kronecker symbol. More generally one can prove that there is no gain of integrability, uniformly with respect to the mesh size h. The same occurs in what concerns the gain of the local regularity. The last pathology is due to the fact that, in contrast with the continuous case, the symbol $p_h(\xi)$ has critical points also at $\pm\pi/h$. These negative results are summarized in the following two theorems.

Theorem 1.3.1 *Let $T > 0$, $q_0 \geq 1$ and $q > q_0$. Then,*

$$\sup_{h>0, \varphi^h \in l^{q_0}(h\mathbf{Z})} \frac{\|S^h(T)\varphi^h\|_{l^q(h\mathbf{Z})}}{\|\varphi^h\|_{l^{q_0}(h\mathbf{Z})}} = \infty \tag{1.8}$$

and

$$\sup_{h>0, \varphi^h \in l^{q_0}(h\mathbf{Z})} \frac{\|S^h(\cdot)\varphi^h\|_{L^1((0,T), l^q(h\mathbf{Z}))}}{\|\varphi^h\|_{l^{q_0}(h\mathbf{Z})}} = \infty. \tag{1.9}$$

Theorem 1.3.2 *Let $T>0$, $q\in[1,2]$ and $s>0$. Then,*

$$\sup_{h>0,\varphi^h\in l^q(h\mathbf{Z})}\frac{\left(h\sum_{j=0}^{1/h}|(D^sS^h(T)\varphi^h)_j|^2\right)^{1/2}}{\|\varphi^h\|_{l^q(h\mathbf{Z})}}=\infty \tag{1.10}$$

and

$$\sup_{h>0,\varphi^h\in l^q(h\mathbf{Z})}\frac{\left(\int_0^T h\sum_{j=0}^{1/h}|(D^sS^h(t)\varphi^h)_j|^2dt\right)^{1/2}}{\|\varphi^h\|_{l^q(h\mathbf{Z})}}=\infty. \tag{1.11}$$

According to these theorems the semi-discrete conservative scheme fails to have uniform dispersive properties with respect to the mesh-size h.

Proof of Theorem 1.3.1. As we mentioned before, this pathological behavior of the semi-discrete scheme is due to the contributions of the frequencies $\pm\pi/2h$. To see this we argue by scaling :

$$\frac{\|S^h(T)\varphi^h\|_{l^q(h\mathbf{Z})}}{\|\varphi^h\|_{l^{q_0}(h\mathbf{Z})}}=\frac{h^{\frac{1}{q}}}{h^{\frac{1}{q_0}}}\frac{\|S^1(T/h^2)\varphi^h\|_{l^q(\mathbf{Z})}}{\|\varphi^h\|_{l^{q_0}(\mathbf{Z})}}, \tag{1.12}$$

reducing the estimates to the case $h=1$.

Using that $p_1(\xi)$ changes convexity at the point $\pi/2$, we choose as initial data a wave packet with its semidiscrete Fourier transform concentrated at $\pi/2$.

We introduce the operator $S_1:\mathcal{S}(\mathbf{R})\to\mathcal{S}(\mathbf{R})$ as

$$(S_1(t)\varphi)(x)=\int_{-\pi}^{\pi}e^{-4it\sin^2\frac{\xi}{2}}e^{ix\xi}\hat{\varphi}(\xi). \tag{1.13}$$

Using the results of Plancherel & Pólya (1937) and Magyar, Stein & Wainger (2002) concerning band-limited functions, i.e., with compactly supported Fourier transform, it is convenient to replace the discrete norms by continuous ones :

$$\sup_{\varphi\in l^{q_0}(\mathbf{Z})}\frac{\|S^1(t)\varphi\|_{l^q(\mathbf{Z})}}{\|\varphi\|_{l^{q_0}(\mathbf{Z})}}\gtrsim\sup_{\operatorname{supp}\hat{\varphi}\subset[-\pi,\pi]}\frac{\|S_1(t)\varphi\|_{L^q(\mathbf{R})}}{\|\varphi\|_{L^{q_0}(\mathbf{R})}}. \tag{1.14}$$

According to this we may consider that x varies continuously in $\mathbf{R}$. To simplify the presentation we set $\psi(\xi)=-4t\sin^2\frac{\xi}{2}+x\xi$. For any interval $[a,b]\subset[-\pi,\pi]$, applying the Mean Value Theorem to $e^{it\psi(\xi)}$, we have

$$\left|\int_a^b e^{i\psi(\xi)}\hat{\varphi}(\xi)d\xi\right|\geq(1-|b-a|\sup_{\xi\in[a,b]}|\psi'(\xi)|)\int_a^b\hat{\varphi}(\xi)d\xi$$

provided that $\hat{\varphi}$ is nonnegative. Observe that

$$\psi'(\xi) = -2t\sin\xi + x \sim -2t\left[1 + O((\xi - \frac{\pi}{2})^2)\right] + x$$

for $\xi \sim \pi/2$. Let ϵ be a small positive number that we shall fix below and $\hat{\varphi}_\epsilon$ supported on the set $\{\xi : \xi - \pi/2 = O(\epsilon)\}$. Then, $|\psi'(\xi)| = O(\epsilon^{-1})$ as long as $x - 2t = O(\epsilon^{-1})$ and $t = O(\epsilon^{-3})$. This implies that

$$\left|\int_{-\pi}^{\pi} e^{-4it\sin^2\frac{\xi}{2} + ix\xi}\hat{\varphi}_\epsilon d\xi\right| \gtrsim \int_{\frac{\pi}{2}-\epsilon}^{\frac{\pi}{2}+\epsilon} \hat{\varphi}_\epsilon(\xi)d\xi.$$

Integrating over $x - 2t = O(\epsilon^{-1})$ we get, for all $t = O(\epsilon^{-3})$,

$$\|S_1(t)\varphi_\epsilon\|_{L^q(\mathbf{R})} \gtrsim \epsilon^{-\frac{1}{q}} \int_{\frac{\pi}{2}-\epsilon}^{\frac{\pi}{2}+\epsilon} \hat{\varphi}_\epsilon(\xi)d\xi. \qquad (1.15)$$

Then,

$$\frac{\|S_1(t)\varphi_\epsilon\|_{L^q(\mathbf{R})}}{\|\varphi_\epsilon\|_{L^{q_0}(\mathbf{R})}} \gtrsim \epsilon^{-\frac{1}{q}} \frac{\int_{\frac{\pi}{2}-\epsilon}^{\frac{\pi}{2}+\epsilon} \hat{\varphi}_\epsilon(\xi)d\xi}{\|\varphi_\epsilon\|_{L^{q_0}(\mathbf{R})}}. \qquad (1.16)$$

We now choose a function φ such that its Fourier transform $\hat{\varphi}$ has compact support and satisfies $\hat{\varphi}(0) > 0$. Then we choose φ_ϵ in the following manner

$$\hat{\varphi}_\epsilon(\xi) = \epsilon^{-1}\hat{\varphi}\left(\epsilon^{-1}(\xi - \frac{\pi}{2})\right).$$

For such φ_ϵ, using the properties of the Fourier transform, we obtain that $\|\varphi_\epsilon\|_{L^{q_0}(\mathbf{R})}$ behaves as ϵ^{-1/q_0} and

$$\frac{\|S_1(t)\varphi_\epsilon\|_{L^q(\mathbf{R})}}{\|\varphi_\epsilon\|_{L^{q_0}(\mathbf{R})}} \gtrsim \epsilon^{-\frac{1}{q}+\frac{1}{q_0}}$$

as long as $t = O(\epsilon^{-3})$.

Finally we choose ϵ such that $\epsilon^{-3} \simeq h^{-2}$. Then, $T/h^2 \sim \epsilon^{-3}$ and the above results imply

$$\begin{aligned} h^{\frac{1}{q}-\frac{1}{q_0}} \sup_{\operatorname{supp}\hat{\varphi}\subset[-\pi,\pi]} \frac{\|S_1(T/h^2)\varphi^h\|_{L^q(\mathbf{R})}dt}{\|\varphi^h\|_{L^{q_0}(\mathbf{R})}} &\gtrsim h^{\frac{1}{q}-\frac{1}{q_0}} h^{\frac{2}{3}(-\frac{1}{q}+\frac{1}{q_0})} \\ &\gtrsim h^{\frac{1}{3}(\frac{1}{q}-\frac{1}{q_0})}. \qquad (1.17) \end{aligned}$$

This, together with (1.12) and (1.14), finishes the proof. □

Proof of Theorem 1.3.2. The proof uses the same ideas as in the case of Theorem 1.3.1 with the difference that we choose wave packets concentrated at π. □

1.4 The Viscous Semi-discretization Scheme

As we have seen in the previous section a simple conservative approximation with finite differences does not reflect the dispersive properties of the LSE. In general, a numerical scheme introduces artificial numerical dispersion, which is an intrinsic property of the scheme and not of the original PDE. A possible remedy is to introduce a dissipative term to compensate the artificial numerical dispersion.

We propose the following viscous semi-discretization of (1.1)

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = ia(h)\mathrm{sgn}(t)\Delta_h u^h, \; t \neq 0, \\ u^h(0) = \varphi^h, \end{cases} \tag{1.18}$$

where $a(h)$ is a positive function which tends to 0 as h tends to 0. We remark that the proposed scheme is a combination of the conservative approximation of the Schrödinger equation and a semidiscretization of the heat equation in a suitable time-scale. More precisely, the scheme

$$\frac{du^h}{dt} = a(h)\Delta_h u^h$$

which underlines in (1.18) may be viewed as a discretization of

$$u_t = a(h)\Delta u,$$

which is, indeed, a heat equation in the appropriate time-scale. The scheme (1.18) generates a semigroup $S_+^h(t)$, for $t > 0$. Similarly one may define $S_-^h(t)$, for $t < 0$. The solution u^h satisfies the following energy estimate

$$\frac{d}{dt}\left[\frac{1}{2}\|u^h(t)\|^2_{l^2(h\mathbf{Z})}\right] = -a(h)\mathrm{sgn}(t)\left[h\sum_{j\in\mathbf{Z}}\left|\frac{u^h_{j+1}(t) - u^h_j(t)}{h}\right|^2\right]. \tag{1.19}$$

In this energy identity the role that the numerical viscosity term plays is clearly reflected. In particular it follows that

$$a(h)\int_{\mathbf{R}} \|D^1 u^h(t)\|^2_{l^2(h\mathbf{Z})}dt \leq \frac{1}{2}\|\varphi^h\|^2_{l^2(h\mathbf{Z})}. \tag{1.20}$$

Therefore in addition to the L^2-stability property we get some partial information on $D^1u^h(t)$ in $l^2(h\mathbf{Z})$ that, despite the vanishing multiplicative factor $a(h)$, gives some extra control on the high frequencies.

The following result holds.

Theorem 1.4.1 *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* $l^{p'}(h\mathbf{Z})$ *into* $l^p(h\mathbf{Z})$ *and there exists some positive constant* $c(p)$ *such that*

$$\|S^h_\pm(t)\varphi^h\|_{l^p(h\mathbf{Z})} \leq c(p)(|t|^{-\alpha(1-\frac{2}{p})} + |t|^{-\frac{1}{2}(1-\frac{2}{p})})\|\varphi^h\|_{l^{p'}(h\mathbf{Z})} \tag{1.21}$$

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

As Theorem 1.4.1 indicates, when $\alpha > 1/2$, roughly speaking, (1.18) reproduces the decay properties of LSE as $t \to \infty$.

Proof of Theorem 1.4.1. We consider the case of $S^h_+(t)$, the other one being similar. We point out that $S^h_+(t)\varphi^h = \exp((i+a(h)\mathrm{sgn}(t))t\Delta_h)\varphi^h$. The term $\exp(a(h)\mathrm{sgn}(t)t\Delta_h)\varphi^h$ represents the solution of the semi-discrete heat equation

$$v^h_t - \Delta_h v^h = 0 \tag{1.22}$$

at time $|t|a(h)$. This shows that, as we mentioned above, the viscous scheme is a combination of the conservative one and the semi-discrete heat equation.

Concerning the semidiscrete approximation (1.22) we have, as in the continuous case, the following uniform (with respect to h) norm decay :

$$\|v^h(t)\|_{l^p(h\mathbf{Z})} \lesssim |t|^{-1/2(1/q-1/p)}\|v^h_0\|_{l^q(h\mathbf{Z})} \tag{1.23}$$

for all $1 \leq q \leq p \leq \infty$. This is a simple consequence of the following estimate (that is obtained by multiplying (1.22) by the test function $|v^h_j|^{p-1}v^h_j$)

$$\frac{d}{dt}\left(\|v^h(t)\|^p_{l^p(h\mathbf{Z})}\right) \leq -c(p)\|\nabla^+|v^h|^{p/2}\|_{l^2(h\mathbf{Z})}$$

and discrete Sobolev inequalities (see Escobedo & Zuazua (1991) for its continuous counterpart).

In order to obtain (1.21) it suffices to consider the case $p' = 1$ and $p' = 2$, since the others follow by interpolation. The case $p' = 2$ is a simple consequence of the energy estimate (1.19). The terms $t^{-\alpha(1-2/p)}$ and $t^{-1/2(1-2/p)}$ are obtained when estimating the high and low frequencies, respectively. The numerical viscosity term contributes to the estimates of the high frequencies. The low frequencies are estimated by applying the Van der Corput Lemma (cf. Stein (1993), Proposition 2, Ch. VIII.§1, p. 332).

We consider the projection operator P^h on the low frequencies $[-\pi/4h, \pi/4h]$ defined by $\widehat{P^h\varphi^h} = \widehat{\varphi^h}\chi_{(-\pi/4h,\pi/4h)}$. Using that

$$S_+^h\varphi^h = e^{it\Delta_h}e^{ta(h)\Delta_h}[P^h\varphi^h + (I-P^h)\varphi^h]$$

it is sufficient to prove that

$$\|e^{it\Delta_h}e^{ta(h)\Delta_h}P^h\varphi^h\|_{l^\infty(\mathbf{Z})} \lesssim \frac{1}{t^{1/2}}\|\varphi^h\|_{l^1(h\mathbf{Z})} \tag{1.24}$$

and

$$\|e^{it\Delta_h}e^{ta(h)\Delta_h}(I-P^h)\varphi^h\|_{l^\infty(\mathbf{Z})} \lesssim \frac{1}{t^\alpha}\|\varphi^h\|_{l^1(h\mathbf{Z})} \tag{1.25}$$

for all $t > 0$, uniformly in $h > 0$. By Young's Inequality it is sufficient to obtain upper bounds for the kernels of the operators involved:

$$K_1^h(t) = \chi_{(-\pi/4h,\pi/4h)}e^{-4it\sin^2(\frac{\xi h}{2})-4ta(h)\sin^2(\frac{\xi h}{2})}$$

and

$$K_2^h(t) = \chi_{(-\pi/h,\pi/h)\setminus(-\pi/4h,\pi/4h)}e^{-4it\sin^2(\frac{\xi h}{2})-4ta(h)\sin^2(\frac{\xi h}{2})}.$$

The second estimate comes from the following

$$\|K_2^h(t)\|_{l^\infty(h\mathbf{Z})} \le \int_{\frac{\pi}{4h}}^{\frac{\pi}{h}} e^{-4t\frac{a(h)}{h^2}\sin^2(\frac{\xi h}{2})}d\xi \lesssim \frac{1}{h}\left(\frac{ta(h)}{h^2}\right)^{-\alpha} \lesssim \frac{1}{t^\alpha}.$$

The first kernel is rewritten as $K_1^h(t) = K_3^h(t) * H^h(ta(h))$, where $K_3^h(t)$ is the kernel of the operator $P^he^{it\Delta_h}$ and H^h is the kernel of the semidiscrete heat equation (1.22). Using the Van der Corput lemma we obtain $\|K_3^h(t)\|_{l^\infty(h\mathbf{Z})} \lesssim 1/\sqrt{t}$. Also by (1.23) we get $\|H^h(ta(h))\|_{l^1(h\mathbf{Z})} \lesssim 1$. Finally by Young's inequality we obtain the desired estimate for $K_1^h(t)$. $\square$

As a consequence of the above theorem, the following TT^* estimate is satisfied.

Lemma 1.4.1 *For $r \ge 2$ and $\alpha \in (1/2, 1]$, there exists a constant $c(r)$ such that*

$$\|(S^h_{\mathrm{sgn}(t)}(t))^* S^h_{\mathrm{sgn}(s)}(s)f^h\|_{l^r(h\mathbf{Z})} \le$$
$$\le c(r)(|t-s|^{-\alpha(1-\frac{2}{r})} + \quad |t-s|^{-1/2(1-\frac{2}{r})})\|f^h\|_{l^{r'}(h\mathbf{Z})}$$

holds for all $t \neq s$.

As a consequence of this, we have the following result.

Theorem 1.4.2 *The following properties hold :*

(i) For every $\varphi^h \in l^2(h\mathbf{Z})$ and finite $T > 0$, the function $S^h_{\mathrm{sgn}(t)}(t)\varphi^h$ belongs to $L^q([-T,T], l^r(h\mathbf{Z})) \cap C([-T,T], l^2(h\mathbf{Z}))$ for every α-admissible pair (q,r). Furthermore, there exists a constant $c(T,r,q)$ depending on $T > 0$ such that

$$\|S^h_{\mathrm{sgn}(\cdot)}(\cdot)\varphi^h\|_{L^q([-T,T],l^r(h\mathbf{Z}))} \leq c(T,r,q)\|\varphi^h\|_{l^2(h\mathbf{Z})}, \tag{1.26}$$

for all $\varphi^h \in l^2(h\mathbf{Z})$ and $h > 0$.

(ii) If (γ,ρ) is an α-admissible pair and $f \in L^{\gamma'}([-T,T], l^{\rho'}(h\mathbf{Z}))$, then for every α-admissible pair (q,r), the function

$$t \mapsto \Phi_f(t) = \int_{\mathbf{R}} S^h_{\mathrm{sgn}(t-s)}(t-s)f(s)ds, \ t \in [-T,T] \tag{1.27}$$

belongs to $L^q([-T,T], l^r(h\mathbf{Z})) \cap C([-T,T], l^2(h\mathbf{Z}))$. Furthermore, there exists a constant $c(T,q,r,\gamma,\rho)$ such that

$$\|\Phi_f\|_{L^q([-T,T],l^r(h\mathbf{Z}))} \leq c(T,q,r,\gamma,\rho)\|f\|_{L^{\gamma'}([-T,T],l^{\rho'}(h\mathbf{Z}))}, \tag{1.28}$$

for all $f \in L^{\gamma'}([-T,T], l^{\rho'}(h\mathbf{Z}))$ and $h > 0$.

Proof All the above estimates follow from Lemma 1.4.1 as a simple consequence of the classical TT^* argument (cf. Cazenave (2003), Ch. 2, Section 3, p. 33). □

We remark that all the estimates are local in time. This is a consequence of the different behavior of the operators $S^h_{\pm}$ at $t \sim 0$ and $t \sim \pm\infty$. Despite their local (in time) character, these estimates are sufficient to prove well-posedness and convergence for approximations of the nonlinear Schrödinger equation. Global estimates can be obtained by replacing the artificial viscosity term $a(h)\Delta_h$ in (1.18) by a higher order one : $\tilde{a}(h)\Delta_h^2$ with a convenient $\tilde{a}(h)$. The same arguments as before ensure the same decay as in (1.21) as $t \sim 0$ and $t \sim \infty$, namely $t^{-\frac{1}{2}(1-\frac{2}{p})}$.

Remark 1.4.1 Using similar arguments one can also show that a uniform (with respect to h) gain of s space derivatives locally in $L^2_{x,t}$ holds for $0 < s < 1/2\alpha - 1/2$. In fact one can prove the following stronger result.

Theorem 1.4.3 *For all $\varphi^h \in l^2(h\mathbf{Z})$ and $0 < s < 1/2\alpha - 1/2$*

$$\sup_{j\in\mathbf{Z}} \int_{-\infty}^{\infty} |(D^s S^h_{\mathrm{sgn}(t)}(t)\varphi^h)_j|^2 dt \lesssim \|\varphi\|^2_{l^2(h\mathbf{Z})} \tag{1.29}$$

holds uniformly in $h > 0$.

This is a consequence of the energy estimate (1.20) for the high frequencies and of dispersive arguments for the low ones (cf. Constantin & Saut (1988) and Kenig, Ponce & Vega (1991)).

1.5 A Viscous Approximation of the NSE

We concentrate on the semilinear NSE equation in $\mathbf{R}$:

$$\begin{cases} iu_t + \Delta u = |u|^p u, \; x \in \mathbf{R}, \; t > 0, \\ u(0,x) = \varphi(x), \; x \in \mathbf{R}. \end{cases} \tag{1.30}$$

It is convenient to rewrite the problem (1.30) in the integral form

$$u(t) = S(t)\varphi - i \int_0^t S(t-s)|u(s)|^p u(s) ds, \tag{1.31}$$

where the Schrödinger operator $S(t) = e^{it\Delta}$ is a one-parameter unitary group in $L^2(\mathbf{R})$ associated with the linear continuous Schrödinger equation. The first result, due to Tsutsumi (1987), on the global existence for L^2-initial data, is the following theorem.

Theorem 1.5.1 *(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 of (1.30) in $C(\mathbf{R}, L^2(\mathbf{R})) \cap L^q_{loc}(\mathbf{R}, L^{p+2}(\mathbf{R}))$ with $q = 4(p+1)/p$ that satisfies the L^2-norm conservation property*

$$\|u(t)\|_{L^2(\mathbf{R})} = \|\varphi\|_{L^2(\mathbf{R})}.$$

This solution depends continuously on the initial condition φ in $L^2(\mathbf{R})$.

Local existence is proved by applying a fixed point argument in the integral formulation (1.31). Global existence holds because of the $L^2(\mathbf{R})$-conservation property which allows excluding finite-time blow-up.

We now consider the following viscous semi-discretization of (1.30):

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = i\,\mathrm{sgn}(t) a(h) \Delta_h u^h + |u^h|^p u^h, t \neq 0, \\ u^h(0) = \varphi^h, \end{cases} \tag{1.32}$$

with $0 \le p < 4$ and $a(h) = h^{2-\frac{1}{\alpha(h)}}$ such that $\alpha(h) \downarrow 1/2$ and $a(h) \to 0$ as $h \downarrow 0$. The following $l^2(h\mathbf{Z})$-norm dissipation law holds:

$$\frac{d}{dt}\left(\frac{1}{2}\|u^h(t)\|^2_{l^2(h\mathbf{Z})}\right) = -a(h)\mathrm{sgn}(t)\left[h\sum_{j\in\mathbf{Z}}\left|\frac{u^h_{j+1}-u^h_j}{h}\right|^2\right]. \tag{1.33}$$

Concerning the well posedness of (1.32) the following holds:

Theorem 1.5.2 *(Ignat and Zuazua (2005a)). Let $p \in (0,4)$ and $\alpha(h) \in (1/2, 2/p]$. Set*

$$\frac{1}{q(h)} = \alpha(h)\left(\frac{1}{2} - \frac{1}{p+2}\right)$$

so 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

$$u^h \in C(\mathbf{R}, l^2(h\mathbf{Z})) \cap L^{q(h)}_{loc}(\mathbf{R}; l^{p+2}(h\mathbf{Z}))$$

of (1.32) which satisfies the following estimates, independently of h:

$$\|u^h\|_{L^\infty(\mathbf{R}, l^2(h\mathbf{Z}))} \le \|\varphi^h\|_{l^2(h\mathbf{Z})} \tag{1.34}$$

and, for all finite $T > 0$,

$$\|u^h\|_{L^{q(h)}([-T,T], l^{p+2}(h\mathbf{Z}))} \le c(T)\|\varphi^h\|_{l^2(h\mathbf{Z})}. \tag{1.35}$$

Sketch of the Proof. The proof uses Theorem 1.4.2 and a standard fixed point argument as in Tsutsumi (1987) and Cazenave (2003) in order to obtain local solutions. Using the a priori estimate (1.33) we obtain a global in time solution.

Let us now address the problem of convergence as $h \to 0$. Given $\varphi \in L^2(\mathbf{R})$, for the semi-discrete problem (1.32) we consider a family of initial data $(\varphi^h_j)_{j\in\mathbf{Z}}$ such that

$$E_h\varphi^h \to \varphi$$

weakly in $L^2(\mathbf{R})$ as $h \to 0$. Here and in the sequel E_h denote the piecewise constant interpolator $E_h : l^2(h\mathbf{Z}) \to L^2(\mathbf{R})$.

The main convergence result is contained in the following theorem.

Theorem 1.5.3 *The sequence $E_h u^h$ satisfies*

$$E_h u^h \overset{\star}{\rightharpoonup} u \text{ in } L^\infty(\mathbf{R}, L^2(\mathbf{R})), \tag{1.36}$$

$$E_h u^h \rightharpoonup u \text{ in } L^s_{loc}(\mathbf{R}, L^{p+2}(\mathbf{R}))\ \forall s < q, \tag{1.37}$$

$$E_h u^h \to u \;\; in \;\; L^2_{loc}(\mathbf{R}\times\mathbf{R}), \tag{1.38}$$

$$|E_h u^h|^p E_h u^h \rightharpoonup |u|^p u \;\; in \;\; L^{q'}_{loc}(\mathbf{R}, L^{(p+2)'}(\mathbf{R})) \tag{1.39}$$

where u is the unique solution of NSE and $2/q = 1/2 - 1/(p+2)$.

Remark 1.5.1 Our method works similarly in the critical case $p = 4$ for small initial data. It suffices to modify the approximation scheme by taking a nonlinear term of the form $|u^h|^{2/\alpha(h)}u^h$ in the semi-discrete equation (1.32) with $a(h) = h^{2-1/\alpha(h)}$ and $\alpha(h) \downarrow 1/2$, $a(h) \downarrow 0$, so that, asymptotically, it approximates the critical nonlinearity of the continuous Schrödinger equation. In this way the critical continuous exponent $p = 4$ is approximated by semi-discrete critical problems.

The critical semi-discrete problem presents the same difficulties as the continuous one. Thus, the initial datum needs to be assumed to be small. But the smallness condition is independent of the mesh-size $h > 0$. More precisely, the following holds.

Theorem 1.5.4 *Let $\alpha(h) > 1/2$ and $p(h) = 2/\alpha(h)$. There exists a constant ϵ, independent of h, such that for all $\|\varphi^h\|_{l^2(h\mathbf{Z})} < \epsilon$, the semi-discrete critical equation has a unique global solution*

$$u^h \in C(\mathbf{R}, l^2(h\mathbf{Z})) \cap L^{p(h)+2}_{loc}(\mathbf{R}, l^{p(h)+2}(h\mathbf{Z})). \tag{1.40}$$

Moreover $u^h \in L^q_{loc}(\mathbf{R}, l^r(h\mathbf{Z}))$ for all $\alpha(h)$- admissible pairs (q,r) and

$$\|u^h\|_{L^q((-T,T),l^r(h\mathbf{Z}))} \le C(q,T)\|\varphi^h\|_{l^2(h\mathbf{Z})}. \tag{1.41}$$

Observe that, in particular, $(3/\alpha(h), 6)$ is an $\alpha(h)$-admissible pair. This allows us to bound the solutions u^h in a space $L^s_{loc}(\mathbf{R}, L^6(\mathbf{R}))$ with $s < 6$. With the same notation as in the subcritical case the following convergence result holds.

Theorem 1.5.5 *When $p = 4$ and under the smallness assumption of Theorem 1.5.4, the sequence Eu^h satisfies*

$$Eu^h \overset{\star}{\rightharpoonup} u \;\; in \;\; L^\infty(\mathbf{R}, L^2(\mathbf{R})), \tag{1.42}$$

$$Eu^h \rightharpoonup u \;\; in \;\; L^s_{loc}(\mathbf{R}, L^6(\mathbf{R}))\, \forall\, s < 6, \tag{1.43}$$

$$Eu^h \to u \;\; in \;\; L^2_{loc}(\mathbf{R}\times\mathbf{R}), \tag{1.44}$$

$$|Eu^h|^{p(h)}|Eu^h| \rightharpoonup |u|^4 u \ \textit{in} \ \ L^{6'}_{loc}(\mathbf{R}, L^{6'}(\mathbf{R})) \tag{1.45}$$

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

1.6 A Two-Grid Scheme

As an alternative to the previous scheme based on numerical viscosity, we propose a two-grid algorithm introduced in Ignat & Zuazua (2005b), which allows constructing conservative and convergent numerical schemes for the nonlinear Schrödinger equation. As we shall see, the two-grid method acts as a preconditioner or filter that eliminates the unwanted high-frequency components from the initial data and nonlinearity. This method is inspired by that used in Glowinski (1992) and Negreanu & Zuazua (2004) in the context of the propagation and control of the wave equation. We emphasize that, by this alternative approach, the purely conservative nature of the scheme is preserved. But, for that to be the case, the nonlinearity needs to be approximated in a careful way.

The method is roughly as follows. We consider two meshes: the coarse one $4h\mathbf{Z}$ of size $4h$, $h > 0$, and the fine one $h\mathbf{Z}$, of size $h > 0$. The computational mesh is the fine one, of size h. The method relies basically on solving the finite-difference semi-discretization (1.4) on the fine mesh $h\mathbf{Z}$, but only for slowly oscillating data and nonlinearity, interpolated from the coarse grid $4h\mathbf{Z}$. As we shall see, the $1/4$ ratio between the two meshes is important to guarantee the convergence of the method. This choice of the mesh-ratio guarantees a particular structure of the data that cancels the two pathologies of the discrete symbol mentioned above. Indeed, a careful Fourier analysis of those initial data shows that their discrete Fourier transforms vanish quadratically at the points $\xi = \pm\pi/2h$ and $\xi = \pm\pi/h$. As we shall see, this suffices to recover the dispersive properties of the continuous model.

To make the analysis rigorous we introduce the space of slowly oscillating sequences (SOS). The SOS on the fine grid $h\mathbf{Z}$ are those which are obtained from the coarse grid $4h\mathbf{Z}$ by an interpolation process. Obviously there is a one to one correspondence between the coarse grid sequences and the space

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

We introduce the extension operator E:

$$(E\psi)((4j+r)h) = \frac{4-r}{4}\psi(4jh) + \frac{r}{4}\psi((4j+4)h), \tag{1.46}$$

for all $j \in \mathbf{Z}$, $r = \overline{0,3}$ and $\psi \in \mathbf{C}_4^{h\mathbf{Z}}$. This associates to each element of $\mathbf{C}_4^{h\mathbf{Z}}$ an SOS on the fine grid. The space of slowly oscillating sequences on the fine grid is as follows

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

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

$$(\Pi\phi)((4j+r)h) = \phi((4j+r)h)\delta_{4r}\, \forall j \in \mathbf{Z}, r = \overline{0,3}, \phi \in \mathbf{C}^{h\mathbf{Z}} \tag{1.47}$$

where δ is Kronecker's symbol. We remark that $E : C_4^{h\mathbf{Z}} \to V_4^h$ and $\Pi : V_4^h \to \mathbf{C}_4^{h\mathbf{Z}}$ are bijective linear maps satisfying $\Pi E = I_{\mathbf{C}_4^{h\mathbf{Z}}}$ and $E\Pi = I_{V_4^h}$, where I_X denotes the identity operator on X. We now define $\tilde{\Pi} = E\Pi : \mathbf{C}^{h\mathbf{Z}} \to V_4^h$, which acts as a smoothing or filtering operator and associates to each sequence on the fine grid a slowly oscillating one. As we said above, the restriction of this operator to V_4^h is the identity.

Concerning the discrete Fourier transform of SOS, by means of explicit computations, one can prove that:

Lemma 1.6.1 *Let $\phi \in l^2(h\mathbf{Z})$. Then,*

$$\widehat{\tilde{\Pi}\phi}(\xi) = 4\cos^2(\xi h)\cos^2\left(\frac{\xi h}{2}\right)\widehat{\Pi\phi}(\xi). \tag{1.48}$$

Remark 1.6.1 One could think on a simpler two-grid construction, using mesh-ratio $1/2$ and, consequently, considering meshes of size h and $2h$. We then get $\widehat{\tilde{\Pi}\varphi}(\xi) = 2\cos^2(\xi h/2)\widehat{\Pi\varphi}(\xi)$. This cancels the spurious numerical solutions at the frequencies $\pm\pi/h$ (see Fig. 1.3), but not at $\pm\pi/2h$. In this case, as we proved in Section 1.3, the Strichartz estimates fail to be uniform on h. Thus instead we choose the ratio between grids to be $1/4$. As the Figure 1.4 shows, the multiplicative factor occurring in (1.48) will cancel the spurious numerical solutions at $\pm\pi/h$ and $\pm\pi/2h$.

As we have proved in Section 1.3, there is no gain (uniformly in h) of integrability of the linear semigroup $e^{it\Delta_h}$. However the linear semigroup has appropriate decay properties when restricted to V_4^h uniformly in $h > 0$. The main results we get are the following.

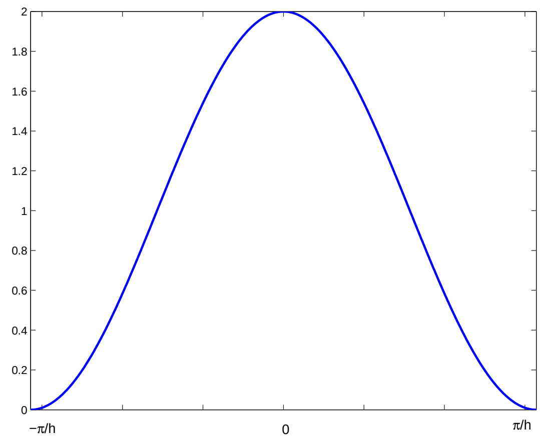

Fig. 1.3. The multiplicative factor $2\cos^2(\xi h/2)$ for the two-grid method with mesh ratio 1/2

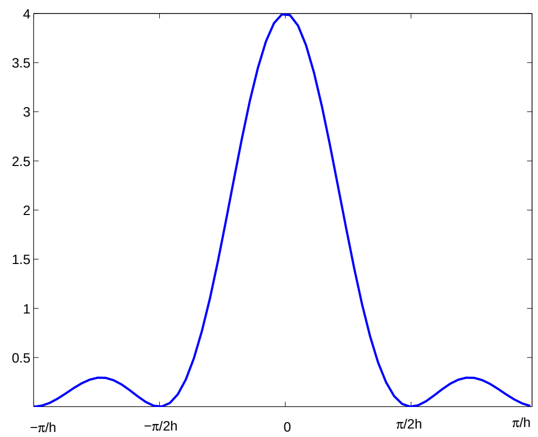

Fig. 1.4. The multiplicative factor $4\cos^2(\xi h)\cos^2\left(\frac{\xi h}{2}\right)$ for the two-grid method with mesh ratio 1/4

Theorem 1.6.1 *Let $p \geq 2$. The following properties hold:*

i) $\|e^{it\Delta_h}\tilde{\Pi}\varphi\|_{l^p(h\mathbf{Z})} \lesssim |t|^{-1/2(1/p'-1/p)}\|\tilde{\Pi}\varphi\|_{l^{p'}(h\mathbf{Z})}$ *for all* $\varphi \in l^{p'}(h\mathbf{Z})$, $h > 0$ *and* $t \neq 0$.

ii) For every sequence $\varphi \in l^2(h\mathbf{Z})$, *the function* $t \to e^{it\Delta_h}\tilde{\Pi}\varphi$ *belongs* *to* $L^q(\mathbf{R}, l^r(h\mathbf{Z})) \cap C(\mathbf{R}, l^2(h\mathbf{Z}))$ *for every admissible pair* (q,r). *Furthermore,*

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

uniformly in $h > 0$.

iii) Let (q,r), $(\tilde{q},\tilde{r})$ *be two admissible pairs. Then,*

$$\left\| \int_{s<t} e^{i(t-s)\Delta_h}\tilde{\Pi}F(s)ds \right\|_{L^q(\mathbf{R},l^r(h\mathbf{Z}))} \lesssim \|\tilde{\Pi}F\|_{L^{\tilde{q}}(\mathbf{R},l^{\tilde{r}}(h\mathbf{Z}))}$$

for all $F \in L^{\tilde{q}}(\mathbf{R}, l^{\tilde{r}}(h\mathbf{Z}))$, *uniformly in* $h > 0$.

Concerning the local smoothing properties we can prove the following result.

Theorem 1.6.2 *The following estimate*

$$\sup_{j\in\mathbf{Z}} \int_{-\infty}^{\infty} \left|(D^{1/2}e^{it\Delta_h}\tilde{\Pi}f)_j\right|^2 dt \lesssim \|\tilde{\Pi}f\|^2_{l^2(h\mathbf{Z})} \tag{1.49}$$

holds for all $f \in l^2(h\mathbf{Z})$, *uniformly in* $h > 0$.

Proof of Theorem 1.6.1. The estimates ii) and iii) easily follow by the classical TT^* argument (cf. Keel & Tao (1998), Cazenave (2003)) once one proves i) with $p' = 1$ and $p' = 2$. The case $p' = 2$ is a consequence of the conservation of energy property. For $p' = 1$, by a scaling argument, we may assume that $h = 1$. The same arguments as in Section 1.4, reduce the proof to the following upper bound for the kernel

$$\|K^1(t)\|_{l^\infty(h\mathbf{Z})} \lesssim \frac{1}{t^{1/2}},$$

where

$$\widehat{K^1(t)} = 4e^{-4it\sin^2\frac{\xi}{2}}\cos^2(\xi)\cos^2\left(\frac{\xi}{2}\right).$$

Using the fact that the second derivative of the symbol $4\sin^2(\xi/2)$ is given by $2\cos\xi$, by means of oscillatory integral techniques (cf. Kenig, Ponce & Vega (1991), Corollary 2.9, p. 46) we get

$$\|K^t\|_{l^\infty(\mathbf{Z})} \lesssim \frac{1}{t^{1/2}}\left\|2|\cos(\xi)|^{3/2}\cos^2\frac{\xi}{2}\right\|_{L^\infty([-\pi,\pi])} \lesssim \frac{1}{t^{1/2}}.$$

$\square$

Proof of Theorem 1.6.2. The estimate (1.49) is equivalent to the following one

$$\sup_{j\in\mathbf{Z}}\int_{-\infty}^{\infty}\left|(e^{it\Delta_h}\tilde{\Pi}f)_j\right|^2 dt \lesssim \|D^{-1/2}\tilde{\Pi}f\|^2_{l^2(h\mathbf{Z})}. \tag{1.50}$$

By scaling we consider the case $h = 1$. Applying the results of Kenig, Ponce & Vega (1991) (Theorem 4.1, p. 54) we get

$$\begin{aligned}\sup_{j\in\mathbf{Z}}\int_{-\infty}^{\infty}\left|(e^{it\Delta_h}\tilde{\Pi}f)_j\right|^2 dt &\lesssim \int_{-\pi}^{\pi}\frac{|\widehat{\Pi f}(\xi)|^2\cos^4\xi\cos^4\frac{\xi}{2}}{|\sin\xi|}\,d\xi\\ &\lesssim \int_{-\pi}^{\pi}\frac{|\widehat{\Pi f}(\xi)|^2}{|\xi|}d\xi \lesssim \|D^{-1/2}f\|^2_{l^2(\mathbf{Z})}.\end{aligned}$$

Observe that the key point in the above proof is that the factor $\cos(\xi/2)$ in the amplitude of the Fourier representation of the initial datum compensates the effects of the critical points of the symbol $\sin^2(\xi/2)$ near the points $\pm\pi$.

□

The results proved in Theorem 1.6.1 i) are plotted in Fig. 1.7. We choose an initial datum as in Fig. 1.6, obtained by interpolation of the Dirac delta: $\Pi u(0) = \delta_0$ (see Fig. 1.5). Figure 1.7 shows the different behavior of the solutions of the conservative and the two-grid schemes. The $l^\infty(\mathbf{Z})$-norm of the solution $u^1(t)$ for the two-grid algorithm behaves like $t^{-1/2}$ as $t\to\infty$, with the decay rate predicted above, while the solutions of the conservative scheme, without the two-grid filtering, decay like $t^{-1/3}$.

1.7 A Conservative Approximation of the NSE

We consider the following semi-discretization of the NSE :

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = \tilde{\Pi}f(u^h),\ t\neq 0,\\ u^h(0) = \tilde{\Pi}\varphi^h,\end{cases} \tag{1.51}$$

where $f(u^h)$ is a suitable approximation of $|u|^p u$ with $0 < p < 4$. In order to prove the global well-posedness of (1.51), we need to guarantee the conservation of the $l^2(h\mathbf{Z})$ norm of solutions, a property that the solutions of NSE satisfy. For that the nonlinear term $f(u^h)$ has to be chosen so that $(\tilde{\Pi}f(u^h), u^h)_{l^2(h\mathbf{Z})} \in \mathbf{R}$. For that to be the case, it is not sufficient to discretize the nonlinearity as for the viscous scheme,

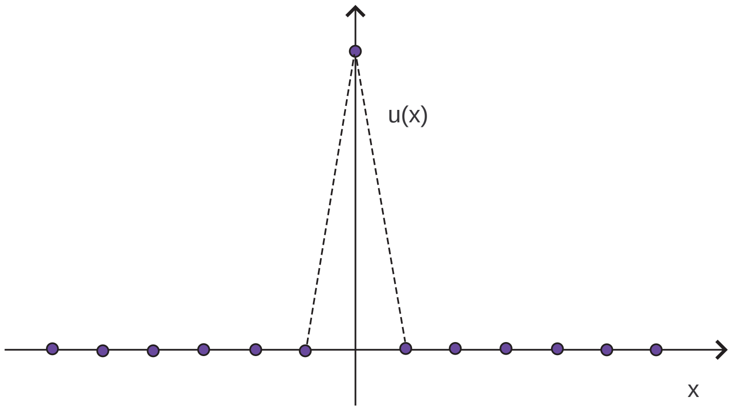

Fig. 1.5. $u^1(0) = \delta_0$

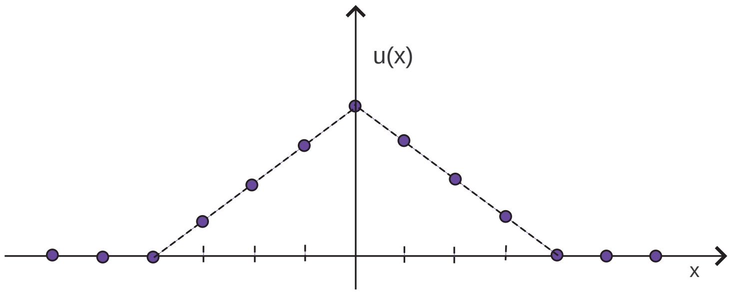

Fig. 1.6. $u^1(0) = E\delta_0$

by simply sampling it on the discrete mesh. A more careful choice is needed. The following result holds.

Theorem 1.7.1 *Let $p \in (0,4)$, $q = 4(p+2)/p$ and $f : \mathbf{C}^{h\mathbf{Z}} \to \mathbf{C}^{h\mathbf{Z}}$ be such that*

$$\|\tilde{\Pi} f(u)\|_{l^{(p+2)'}(h\mathbf{Z})} \lesssim \||u|^p u\|_{l^{(p+2)'}(h\mathbf{Z})} \tag{1.52}$$

and

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

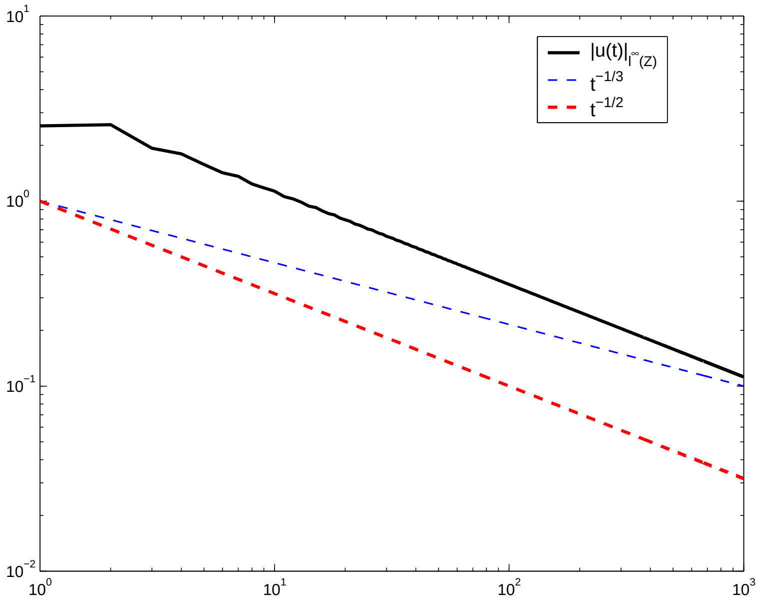

Fig. 1.7. Log-log plot of the time evolution of the l^{∞} norm of $u^{1}(t)$

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

$$u^h \in C(\mathbf{R}, l^2(h\mathbf{Z})) \cap L^q_{loc}(\mathbf{R}; l^{p+2}(h\mathbf{Z})) \tag{1.53}$$

of (1.51) which satisfies the estimates

$$\|u^h\|_{L^\infty(\mathbf{R},l^2(h\mathbf{Z}))} \leq \|\tilde{\Pi}\varphi\|_{l^2(h\mathbf{Z})} \tag{1.54}$$

and

$$\|u^h\|_{L^q(I,l^{p+2}(h\mathbf{Z}))} \leq c(I)\|\tilde{\Pi}\varphi\|_{l^2(h\mathbf{Z})} \tag{1.55}$$

for all finite intervals I*, where the above constants are independent of* h*.*

Remark 1.7.1 The conditions above on the nonlinearity are satisfied if one chooses

$$(f(u^h))_{4j} = g\left((u^h_{4j} + \sum_{r=1}^{3} \frac{4-r}{4}(u^h_{4j+r} + u^h_{4j-r}))/4\right); \quad g(s) = |s|^p s. \tag{1.56}$$

With this choice it is easy to check that (1.52) holds with $C > 0$ independent of $h > 0$. Furthermore $(\tilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})} \in \mathbf{R}$ since

$$
\begin{aligned}
& (\tilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})} = \\
= \;& h \sum_{r=0}^{3} \sum_{j\in\mathbf{Z}} \left(\frac{4-r}{4} (f(u^h))_{4j} + \frac{r}{4} (f(u^h))_{4j+4} \right) \overline{u}^h_{4j+r} \\
= \;& h \sum_{j\in\mathbf{Z}} (f(u^h))_{4j} \left(\sum_{r=0}^{3} \frac{4-r}{4} \overline{u}^h_{4j+r} + \sum_{r=0}^{3} \frac{r}{4} \overline{u}^h_{4j+r-4} \right) \\
= \;& h \sum_{j\in\mathbf{Z}} g \left((u^h_{4j} + \sum_{r=1}^{3} \frac{4-r}{4} (u^h_{4j+r} + u^h_{4j-r}))/4 \right) \\
& \times (\overline{u}^h_{4j} + \sum_{r=1}^{3} \frac{4-r}{4} (\overline{u}^h_{4j+r} + \overline{u}^h_{4j-r})).
\end{aligned}
$$

Proof of Theorem 1.7.1. Local existence and uniqueness are a consequence of the Strichartz estimates (Theorem 1.6.1) and of a fixed point argument. The fact that $(\tilde{\Pi} f(u^h), u^h)_{l^2(h\mathbf{Z})}$ is real guarantees the conservation of the discrete energy $h \sum_{j\in\mathbf{Z}} |u_j(t)|^2$. This allows excluding finite-time blow-up. $\square$

The main convergence result is the following

Theorem 1.7.2 *Let u^h be the unique solution of (1.51) with discrete initial data φ^h such that $E_h\varphi^h \rightharpoonup \varphi$ weakly in $L^2(\mathbf{R})$. Then, the sequence $E_h u^h$ satisfies*

$$E_h u^h \overset{\star}{\rightharpoonup} u \text{ in } L^\infty(\mathbb{R}, L^2(\mathbf{R})), \tag{1.57}$$

$$E_h u^h \rightharpoonup u \text{ in } L^q_{loc}(\mathbb{R}, L^{p+2}(\mathbf{R})), \tag{1.58}$$

$$E_h u^h \to u \text{ in } L^2_{loc}(\mathbb{R} \times \mathbf{R}), \tag{1.59}$$

$$E_h \tilde{\Pi} f(u^h) \rightharpoonup |u|^p u \text{ in } L^{q'}_{loc}(\mathbb{R}, L^{(p+2)'}(\mathbf{R})) \tag{1.60}$$

where u is the unique solution of NSE and $2/q = 1/2 - 1/(p+2)$.

The critical nonlinearity $p = 4$ may also be handled by the two-grid algorithm. In this case one can take directly $p = 4$ in the semi-discrete scheme since the two-grid algorithm guarantees the dispersive estimates to be true for all 1/2-admissible pairs.

1.8 Open Problems

- **Time Splitting Methods.** In Besse, Bidégaray & Descombes (2002), (see also Sanz-Serna & Calvo (1994), Descombres & Schatzman (2002)) the authors consider the NSE with initial data in $H^2(\mathbf{R}^2)$ and the nonlinear term $|u|^2u$. A time splitting method is used in order to approximate the solution. More precisely, the nonlinear Schrödinger equation is split into the flow X^t generated by the linear Schrödinger equation
$$\begin{cases} v_t - i\Delta v = 0,\ x \in \mathbf{R}^2,\ t > 0, \\ v(0,x) = v_0(x),\ x \in \mathbf{R}^2. \end{cases} \tag{1.61}$$
and the flow Y^t for the differential equation
$$\begin{cases} w_t - i|w|^2 w = 0,\ x \in \mathbf{R}^2,\ t > 0, \\ w(0,x) = w_0(x),\ x \in \mathbf{R}^2. \end{cases} \tag{1.62}$$
One can then approximate the flow of NSE by combining the two flows X^t and Y^t using some of the classical splitting methods: the Lie formula $Z_L^t = X^tY^t$ or the Strang formula $Z_S^t = X^{t/2}Y^tX^{t/2}$. In Besse, Bidégaray & Descombes (2002) the convergence of these methods is proved for initial data in $H^2(\mathbf{R}^2)$. Note however that the nonlinearity $|u|^2u$ is locally Lipschitz in $H^2(\mathbf{R}^2)$. Consequently this nonlinearity in this functional setting can be dealt with by means of classical energy methods, without using the Strichartz type estimate.
  A possible problem for future research is to replace the above equations (1.61), (1.62), which are continuous in the variable x, by discrete ones and to analyze the convergence of the splitting method for the initial data in $L^2(\mathbf{R})$. As we saw in Section 1.3 the simpler approximation of (1.61) by finite differences does not have the dispersive properties of the continuous model. It is then natural to consider one of the two remedies we have designed: to add numerical viscosity or to regularize the initial data by a two grid algorithm. The convergence of the splitting algorithm is open because of the lack of dispersion of the ODE (1.62) and its semi-discretizations.
- **Discrete Transparent Boundary Conditions.** In Arnold, Ehrhardt & Sofronov (2003) the authors introduce a discrete transparent boundary condition for a Crank–Nicolson finite difference discretization of the Schrödinger equation. The same ideas allow constructing similar DTBC for various numerical approximations of the LSE. It would be interesting to study the dispersive properties of these approximations by means of the techniques of Markowich & Poupaud

(1999) based on microlocal analysis. Supposing that the approximation fails to have the appropriate dispersive properties, one could apply the methods presented here in order to recover the dispersive properties of the continuous model.

- **Fully Discrete Schemes.** It would be interesting to develop a similar analysis for fully discrete approximation schemes. We present two schemes, one which is implicit and the other one which is explicit in time. The first one:

$$i\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{(\Delta x)^2}=0,\ n\geq 0,\ j\in\mathbf{Z}, \tag{1.63}$$

  introduces time viscosity and consequently has the right dispersive properties. The second one is conservative and probably will present some pathologies. As an example we choose the following approximation scheme:

$$i\frac{u_j^{n+1}-u_j^{n-1}}{2\Delta t}+\frac{u_{j+1}^{n}-2u_j^{n}+u_{j-1}^{n}}{(\Delta x)^2}=0,\ n\geq 1,\ j\in\mathbf{Z}. \tag{1.64}$$

  In this case it is expected that the dispersive properties will not hold for any Courant number $\lambda=\Delta t/(\Delta x)^2$ which satisfies the stability condition. Giving a complete characterization of the fully discrete schemes satisfying the dispersive properties of the continuous Schrödinger equation is an open problem.

- **Bounded Domains.** In Bourgain (1993) the LSE is studied on the torus $\mathbf{R}/\mathbf{Z}$ and the following estimates are proved :

$$\|e^{it\Delta}\varphi\|_{L^4(\mathbf{T}^2)}\lesssim\|\varphi\|_{L^2(\mathbf{T})}. \tag{1.65}$$

  This estimate allows one to show the well posedness of a NSE on $\mathbf{T}^2$. As we prove in Ignat (2006), in the case of the semidiscrete approximations, similar l^2_x-$L^4_t l^4_x$ estimates fail to be uniform with respect to the mesh size Δx. It is an open problem to establish what is the complete range of (q,r) (if any) for which the estimates l^2_x-$L^q_t l^r_x$ are uniform with respect to the mesh size. It is then natural to consider schemes with numerical viscosity or with a two-grid algorithm.

  More recently, the results by Burq, Gérard and Tzvetkov (2004) show Strichartz estimates with loss of derivatives on compact manifolds without boundary. The corresponding results on the discrete level remain to be studied.

- **Variable Coefficients.** In Banica (2003) the global dispersion and the Strichartz inequalities are proved for a class of one-dimensional

Schrödinger equations with step-function coefficients having a finite number of discontinuities. Staffilani & Tataru (2002) proved the Strichartz estimates for C^2 coefficients. As we proved in Section 1.3, even in the case of the approximations of the constant coefficients, the Strichartz estimates fail to be uniform with respect to the mesh size h. It would be interesting to study if the two remedies we have presented in this article are also efficient for a variable-coefficient problem.

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