Dispersive properties of a viscous numerical scheme for the Schrödinger equation

Propriétés dispersives d'un schéma numeríque visqueux pour l'équation de Schrödinger

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Abstract

In this work we study the dispersive properties of the numerical approximation schemes for the free Schrödinger equation. We consider finite-difference space semi-discretizations. We first show that the standard conservative scheme does not reproduce at the discrete level the properties of the continuous Schrödinger equation. This is due to high frequency numerical spurious solutions. In order to damp out these high-frequencies and to reflect the properties of the continuous problem we add a suitable extra numerical viscosity term at a convenient scale. We prove that the dispersive properties of this viscous scheme are uniform when the mesh-size tends to zero. Finally we prove the convergence of this viscous numerical scheme for a class of nonlinear Schrödinger equations with nonlinearities that may not be handeled by standard energy methods and that require the so-called Strichartz inequalities. *To cite this article: Liviu I. Ignat, Enrique Zuazua, C. R. Acad. Sci. Paris, Ser. I,*

Résumé

Dans cette Note on étudié les propriétés dispersives des schémas d'approximation numérique de l'équation de Schrödinger. On considère des approximations semi-discretes en différences finies. Nous démontrons d'abord que le schéma conservatif habituel ne reproduit pas les propriétés dispersives, uniformemet par rapport au pas du maillage. Ceci est du aux hautes fréquences numériques artificielles. On introduit donc un schéma d'approximation visqueux dissipant ces hautes fréquences et l'on montre qu'il possède des propriétés de dispersivité uniformes par rapport au pas du maillage. Nous appliquons ce schéma à l'approximation numérique des équations de Schrödinger non-linéaires. On démontre la convergence dans la classe de non-linéarités dont l'analyse, au niveau de l'équation de Schrödinger continue, a besoin des inegalités de Strichartz. *Pour citer cet article : Liviu I. Ignat, Enrique Zuazua, C. R. Acad. Sci. Paris, Ser. I,*

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Dans cette Note on analyse les propriétés dispersives de quelques schémas semi-discrets en différences finies pour l'approximation numérique du problème de Cauchy pour l'équation de Schrödinger linéaire (ESL). Pour fixer les idées et simplifier l'exposé on se place dans le cas d'une dimension d'espace mais notre analyse et résultats sont aussi valables dans le cas multi-dimensionnel.

On considère d'abord le schéma conservatif semi-discret classique. On démontre que lorsque le pas du maillage h tend vers zéro, ce schéma ne possède pas les propriétés dispersives de l'équation de Schrödinger garantissant un gain d'intégrabilité espace-temps et d'1/2 dérivée en espace localement en $L^2_{x,t}$. La preuve utilise la transformée de Fourier discrète (TDF) et le fait que le symbole du schème semi-discret perd la convexité et monotonie stricte du symbole du laplacien continu. Elle se base sur une construction explicite en paquets d'ondes localisées autour des fréquences où la convexité et monotonie sont perdues.

Donc, même si le schéma converge au sens de la théorie L^2 classique il ne reproduit pas les propriétés dispersives de ESL. Par conséquent il ne garantit pas la convergence pour les équations non-linéaires (ESNL) où l'analyse exige des inégalités de type Strichartz ([C],[Ts]).

Nous introduisons ensuite un schéma nouveau avec un terme de viscosité numérique à une échelle appropriée, évanescent lorsque $h \to 0$. Le schéma converge au sens de la théorie L^2. En outre on montre qu'il reproduit, uniformément par rapport au paramètre h, les propriétés dispersives de ESL. La preuve suit un argument assez intuitif. La viscosité numerique amortit les hautes fréquences. Les basses fréquences, ayant un comportement semblable à celles de l'ESL, peuvent se traiter par des arguments assez classiques inspirés du lemme de la Phase Stationnaire.

Finalement on applique ce schème visqueux à l'approximation numérique de l'ESNL avec non-linéarité répulsive et exposant $0 < p < 4$. L'existence et unicité de la solution a été démontrée dans [Ts] à l'aide des inégalités de Strichartz, par un argument de point fixe. Nous démontrons la convergence des solutions numériques visqueuses.

Le cas critique $p = 4$ reste ouvert.

Nos techniques s'appliquent aussi dans le cas de plusieures variables d'espace.

1. Introduction

Let us to consider the 1-d linear Schrödinger Equation (LSE) in the whole line

$$iu_t + u_{xx} = 0,\ x \in \mathbf{R},\ t > 0; \qquad u(0,x) = \varphi(x),\ x \in \mathbf{R}. \tag{1}$$

This 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 conservation of the L^2-norm $\|u\|_{L^2(\mathbf{R})} = \|\varphi\|_{L^2(\mathbf{R})}$, together with the classical estimate $|u(t,x)| \leq (4\pi|t|)^{-1/2}\|\varphi\|_{L^1(\mathbf{R})}$, leads, by Riesz-Thorin interpolation theorem (see [BL]), to the following result : $\|S(t)\varphi\|_{L^p(\mathbf{R})} \leq t^{-(\frac{1}{2}-\frac{1}{p})}\|\varphi\|_{L^{p'}(\mathbf{R})}$, for all $p \geq 2$ and $t \neq 0$. More refined space-time estimates known as the *Strichartz inequalities* 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 satisfies $2/q = \alpha(1/2 - 1/r)$. Also a local gain of 1/2 space derivate occurs in $L^2_{x,t}$. These properties are not only relevant for a better understanding of the dynamics of the linear system but also to derive well-posedness results for nonlinear Schrödinger equations ([C],[Ts]).

Our main purpose in this paper is to analyze whether the numerical approximation schemes for (1) have the same dispersive properties, uniformly with respect to the mesh-size h. Let us first consider the finite-difference conservative numerical scheme

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

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 the classical second order finite difference approximation of $\partial_x^2 : (\Delta_h u)_j = (u_{j+1} - 2u_j + u_{j-1})/h^2$.

This scheme satisfies the classical properties of consistency and stability which imply the L^2 convergence. The same convergence results hold for semilinear equations $iu_h + u_{xx} = f(u)$(NLE) provided that the nonlinearity f is globally Lipshitz. We refer to [C] for a survey of the important progresses done in this field. But, as proved in [Ts], the NLE is also well-posed for some nonlinearities that grow superlinearly at infinity. This well-posedness result may not 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 on the mesh-size parameter $h \to 0$.

In this article we first prove that this conservative scheme (2) fails to have those uniform dispersive properties. We then introduce a viscous numerical scheme for which the estimates are uniform. This allows proving convergence for the NSEE as well.

We remark that there are *slight* 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 fulfill. As we will prove, these pathologies will affect the dispersive properties of the semi-discrete scheme.

Our analysis uses the discrete Fourier transform (DFT) at the scale h (see [**?**] for more details) defined by $\hat{u}^h = h\sum_{j\in\mathbf{Z}} e^{ijh\xi}u_j$.

Let us define the Banach spaces of sequences $l_h^p(\mathbf{Z})$ as follows

$$l_h^p(\mathbf{Z}) = \{\{c_k\} : \|c_k\|^p_{l_h^p(\mathbf{Z})} = h\sum_{k\in\mathbf{Z}} |c_k|^p < \infty\}.$$

We will also make use of a discrete version of fractional differentiation. For $\varphi^h \in l_h^2(\mathbf{Z})$ and $0 \le s < 1$ we define $(D^s\varphi^h)_j = \int_{-\pi/h}^{\pi/h} |\xi|^s \hat{\varphi}^h(\xi) e^{ij\xi h} d\xi$.

Our first results are of negative nature and read as follows :

Theorem 1.1 *Let $T > 0$, $q_0 \ge 1$ and $q > q_0$. Then*

$$\sup_{h>0,\varphi^h\in l_h^{q_0}(\mathbf{Z})} \frac{\|S^h(T)\varphi^h\|_{l_h^q(\mathbf{Z})}}{\|\varphi^h\|_{l_h^{q_0}(\mathbf{Z})}} = \infty \;\; \textit{and} \;\; \sup_{h>0,\varphi^h\in l_h^{q_0}(\mathbf{Z})} \frac{\|S^h(\cdot)\varphi^h\|_{L^1((0,T),l_h^q(\mathbf{Z}))}}{\|\varphi^h\|_{l_h^{q_0}(\mathbf{Z})}} = \infty. \tag{3}$$

Theorem 1.2 *Let $T > 0$, $q \in [1, 2]$ and $s > 0$. Then*

$$\sup_{h>0,\varphi^h\in l_h^q(\mathbf{Z})} \frac{\left(h\sum_{j=1}^{1/h} |(D^sS^h(T)\varphi^h)_j|^2\right)^{1/2}}{\|\varphi^h\|_{l_h^q(\mathbf{Z})}} = \infty \tag{4}$$

and

$$\sup_{h>0,\varphi^h\in l_h^q(\mathbf{Z})} \frac{\left(\int_0^T h\sum_{j=1}^{1/h} |(D^sS^h(t)\varphi^h)_j|^2 dt\right)^{1/2}}{\|\varphi^h\|_{l_h^q(\mathbf{Z})}} = \infty. \tag{5}$$

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

Sketch of the Proofs. First, using that $p_h(\xi)$ changes convexity at the point $\pi/2h$, we choose as initial data a family of wave packets $\{\varphi^h\}$ with DFT concentrated on $\pi/2h$. For the second theorem we choose initial data with DFT concentrated on π/h. The results are obtained by a simple application of the Stationary Phase Lemma.

2. The viscous semi-discretization scheme

As we have seen in the previous section a simple conservative approximation with finite differences does not reflect the properties of the dispersive LSE. In general, a numerical scheme introduces artificial numerical dispersion, which is an intrinsic property of the scheme and not of the original problem. One remedy is to introduce a dissipative term to compensate the artificial numerical dispersion. We propose the following viscous semi-discretization of (1)

$$i\frac{du^h}{dt} + \Delta_h u^h = ia(h)\text{sgn}(t)\Delta_h u^h,\ t \neq 0; \qquad u^h(0) = \varphi^h, \tag{6}$$

where $a(h)$ is a positive function which tends to 0 as h tends to 0. This scheme 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

$$\tfrac{d}{dt}[\tfrac{1}{2}\|u^h(t)\|^2_{l^2_h(\mathbf{Z})}] = -a(h)[h\textstyle\sum_{j\in\mathbf{Z}}\left|\frac{u^h_{j+1}(t)-u^h_j(t)}{h}\right|^2]. \tag{7}$$

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

$$a(h)\textstyle\int_{\mathbf{R}}\|D^1u^h(t)\|^2_{l^2_h(\mathbf{Z})}dt \leq \tfrac{1}{2}\|\varphi^h\|^2_{l^2_h(\mathbf{Z})}. \tag{8}$$

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 holds :

Theorem 2.1 *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*

$$\|S^h_\pm(t)\varphi^h\|_{l^p_h(\mathbf{Z})} \leq c(p)(|t|^{-\alpha(1-\frac{2}{p})} + |t|^{-\frac{1}{2}(1-\frac{2}{p})})\|\varphi^h\|_{l^{p'}_h(\mathbf{Z})} \tag{9}$$

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

As Theorem 2.1 indicates, when $\alpha > 1/2$, roughly speaking, (6) reproduces the decay properties of LSE.

We now introduce the family of operators $\mathcal{T}^h(t) = S^h_{\text{sgn}(t)}(t)$. The following TT^* estimate is satisfied :

Lemma 2.2 *For $r \geq 2$ and $\alpha \in (1/2,1]$, there exists a constant $c(r)$ such that*

$$\|\mathcal{T}^h(t)^*\mathcal{T}^h(s)f^h\|_{l^r_h(\mathbf{Z})} \leq c(r)|t-s|^{-\alpha(1-\frac{2}{r})}\|f^h\|_{l^{r'}_h(\mathbf{Z})} \tag{10}$$

holds for all $t \neq s$ with $|t-s| \leq 1$.

Theorem 2.3 *The following properties hold :*

(i) For every $\varphi^h \in l^2_h(\mathbf{Z})$ and finite $T > 0$, the function $t \to \mathcal{T}^h(t)\varphi^h$ 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

$$\|T^h(\cdot)\varphi^h\|_{L^q([-T,T],l^r(\mathbf{Z}))} \leq c(T,r,q)\|\varphi^h\|_{l^2_h(\mathbf{Z})},\ \forall\, \varphi^h \in l^2_h(\mathbf{Z}),\ \forall\, h>0. \tag{11}$$

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

$$t \mapsto \Phi_f(t) = \int_0^t T^h(t-s)f(s)ds,\ \ t\in[-T,T] \tag{12}$$

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

$$\|\Phi_f\|_{L^q([-T,T],l^r_h(\mathbf{Z}))} \leq c(T,q,r,\gamma,\rho)\|f\|_{L^{\gamma'}([-T,T],l_h^{\rho'}(\mathbf{Z}))},\ \forall\, f\in L^{\gamma'}([-T,T], l_h^{\rho'}(\mathbf{Z})),\ \forall\, h>0. \tag{13}$$

Sketch of the Proof. We remark that $T^h(t)\varphi^h = \exp((i+a(h)\mathrm{sgn}(t))t\Delta_h)\varphi^h$. The term $\exp(a(h)\mathrm{sgn}(t)t\Delta_h)\varphi^h$ represents the solution of semi-discrete heat equation $\frac{\partial v^h}{\partial t} = \Delta_h v^h$ at time $ta(h)$. This shows that, rougly speaking, the viscous scheme is a combination of the conservative one and the semi-discrete heat equation.

To obtain Lemma 2.2 we use (9) and estimates of the $l^1_h(\mathbf{Z})$-norm of the solution v_h of the discrete heat equation : for all $1\leq q\leq p\leq\infty$ there is a constant $c(p,q)$ such that for all $t\neq 0$, $\|v^h(t)\|_{l^p_h(\mathbf{Z})} \leq c(p,q)|t|^{-1/2(1/q-1/p)}\|v^h(0)\|_{l^q_h(\mathbf{Z})}$ uniformly in h.

In Theorem 2.1 the terms $t^{-\alpha(1-2/p)}$ and $t^{-1/2(1-2/p)}$ are obtained when estimating the high, respectively the low frequencies. The numerical viscosity term gives estimates for the high frequencies. The low frequencies are estimated by the by Van der Corput Lemma (see [Ste]).

The estimates (11) and (13) follow from (10) as a simple consequence of the clasical TT^* argument (see [C]).

Remark 1 Using similar arguments one can also show that an uniform (with respect to h) gain of s space derivatives locally in $L^2_{x,t}$ holds for $0<s<1/2$. This is a consequence of the energy estimate (8) for the high frequencies and of dispersive arguments for the low ones (see [CS])

3. Application to NSE

We concentrate on the semilinear NSE equation in $\mathbf{R}$ with repulsive power law nonlinearity :

$$iu_t + \Delta u = |u|^p u,\ x\in\mathbf{R},\ t>0; \qquad u(0,x)=\varphi(x),\ x\in\mathbf{R}. \tag{14}$$

As proved in [Ts], (14) is globally well posed for all $\varphi\in L^2(\mathbf{R})$ and $p\in[0,4)$.

We consider the following viscous semi-discretization

$$i\frac{du^h}{dt} + \Delta_h u^h = i\mathrm{sgn}(t)a(h)\Delta_h u^h + |u^h|^p u^h, t\neq 0; \quad u^h(0)=\varphi^h, \tag{15}$$

with $0\leq p<4$ and $a(h) = h^{2-\frac{1}{\alpha(h)}}$ such that $\alpha(h)\downarrow 1/2$ and $a(h)\to 0$ as $h\downarrow 0$. Concerning the well posedness of (15) we can prove :

Theorem 3.1 *Let $p\in(0,4)$ and $\alpha(h)\in(1/2,2/p]$. Set $2/q(h) = \alpha(h)(1/2-1/(p+2))$ 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 (15) which satisfies the following estimates

$$\|u^h\|_{L^\infty(\mathbf{R},l^2_h(\mathbf{Z}))} \leq \|\varphi^h\|_{l^2_h(\mathbf{Z})} \text{ and } \|u^h\|_{L^{q(h)}([-T,T],l^{p+2}_h(\mathbf{Z}))} \leq c(T)\|\varphi^h\|_{l^2_h(\mathbf{Z})} \tag{16}$$

for all finite $T > 0$, where the above constants are independent of h.

Sketch of the Proof. The proof uses Theorem 2.3 and a standard fix point argument as in [C], [Ts].

In the sequel we consider the piecewise constant interpolator E_h. We choose $(\varphi^h_j)_{j\in\mathbf{Z}}$ an approximation of the initial data $\varphi \in L^2(\mathbf{R})$ such that $E\varphi^h \rightharpoonup \varphi$ weakly in $L^2(\mathbf{R})$.

The main convergence result is the following

Theorem 3.2 *The sequence Eu^h satisfies*

$$Eu^h \overset{\star}{\rightharpoonup} u \text{ in } L^\infty(\mathbf{R}, L^2(\mathbf{R})), \tag{17}$$

$$Eu^h \rightharpoonup u \text{ in } L^s_{loc}(\mathbf{R}, L^{p+2}(\mathbf{R})), \forall\, s < q, \tag{18}$$

$$Eu^h \to u \text{ in } L^2_{loc}(\mathbf{R}\times\mathbf{R}), \tag{19}$$

$$|Eu^h|^p Eu^h \to |u|^p u \text{ in } L^{q'}_{loc}(\mathbf{R}, L^{(p+2)'}(\mathbf{R})) \tag{20}$$

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

Sketch of the Proof. Using the result in Remark 1 above on the gain of s-derivatives and a fixed point argument we first prove the existence of a positive s, independent by h, such that $\|Eu^h\|_{L^2(\mathbf{R},H^s_{loc}(\mathbf{R}))} \leq \|\varphi^h\|_{l^2_h(\mathbf{Z})}$. Then, by a compactness argument (see [Si]), we can extract a subsequence converging locally strongly in $L^1_{x,t}$. This, together with the uniform (with respect to h) estimates of Theorem 3.1, suffices to obtain the stated convergence results. In particular, it suffices to pass to the limit in the nonlinear term and to identify the limit as the solution of NSE.

Remark 2 The limit case $p = 4$ can not be treated by these arguments and it constitutes an open problem.

Remark 3 The techniques and results of this paper extend to the LSE and NSE in several space dimensions.

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Références

[BL] J. Bergh, J. Löfström, *Interpolation Spaces, An Introduction*, Springer Verlag, 1976.

[C] T. Cazenave, *Semilinear Schrödinger Equations*, Courant Lecture Notes, 10, 2003.

[CS] P. Constantin and J. Saut, *Local smoothing properties of dispersive equations,* J. Am. Math. Soc., **1**(2), 413–439, 1988.

[Si] J. Simon, *Compact sets in the space $L^p(0,T;B)$.* Ann. Mat. Pura Appl. (4), **146**, 65-96, 1987.

[Ste] E. Stein, *Harmonic analysis : real-variable methods, orthogonality, and oscillatory integrals*, Monographs in Harmonic Analysis, III, Princeton University Press, 1993.

[Str] R. S. Strichartz, *Restrictions of Fourier transforms to quadratic surfaces and decay of solutions of wave equations,* Duke Math. J., **44**, 705–714, 1977.

[Ts] Y. Tsutsumi, *L^2-solutions for nonlinear Schrödinger equations and nonlinear groups,* Funkc. Ekvacioj, Ser. Int., **30**,115–125, 1987.