Dispersive Numerics[1]

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[1]Based on joint work with L.Ignat

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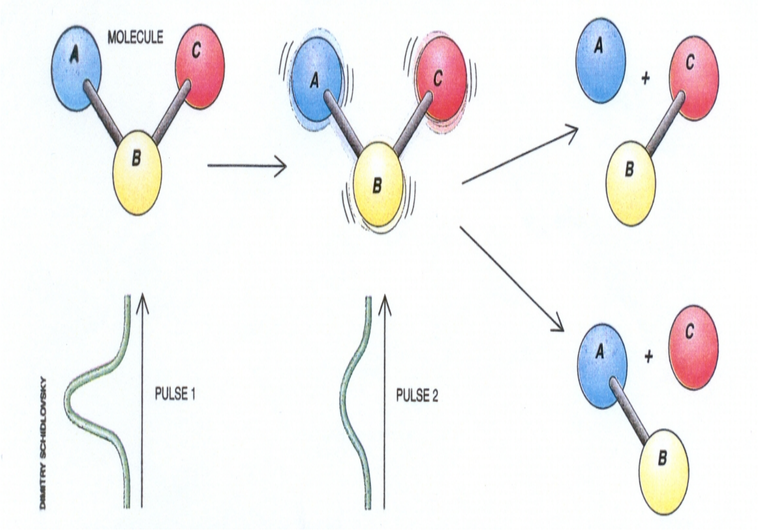

Brumer, Paul, Shapiro, Moshe, Laser Control of Chemical Reactions, Scientific American, 0036-8733, March 1, 1995, Vol. 272, Issue 3.

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to the explanation of the main features of complex atomic systems without too much computations.

Dirac, 1929.

Yousef Saad, James R. Chelikowsky & Suzanne M. Shontz, Numerical Methods for Electronic Structure Calculations of Materials, SIAM REVIEW Vol. 52, No. 1, pp. 354.

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To build convergent numerical schemes for nonlinear PDE of dispersive type: SCHRÖDINGER EQUATION.
Similar problems for other dispersive equations: Korteweg-de-Vries, wave equation, ...

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

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

This has been done succesfully for the PDE models.
What about Numerical schemes?

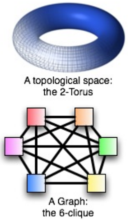
FROM FINITE TO INFINITE DIMENSIONS IN PURELY CONSERVATIVE SYSTEMS.....

UNDERLYING MAJOR PROBLEM:

Reproduce in the computer the dynamics in Continuum and Quantum Mechanics, avoiding spurious numerical solutions.

For this we need to adapt at the discrete numerical level the techniques developed in the continuous context.

WARNING! NUMERICS = CONTINUUM + (POSSIBLY) SPURIOUS



This issue is relevant in **numerical analysis** but also in modeling were the discussion between **continuous versus discrete** models is relevant.

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The appropriate functional setting depends on the model under consideration on a subtle manner.

Consider:

$$\frac{du}{dt}(t) = Au(t), \quad t \geq 0; \quad u(0) = u_0.$$

A an unbounded operator in a Hilbert (or Banach) space H, with domain $D(A) \subset H$. The solution is given by

$$u(t) = e^{At}u_0.$$

Semigroup theory provides conditions under which e^{At} is well defined.

Roughly A needs to be *maximal* ($A + I$ is invertible) and *dissipative* ($A \leq 0$).

Most of the *linear* PDE from Mechanics enter in this general frame: wave, heat, Schrödinger equations,...

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

$$u_t(t) = Au(t) + f(u(t)), \quad t \geq 0; \quad u(0) = u_0.$$

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

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

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

But, often in applications, the property that $f : H \to H$ is locally Lipschitz FAILS.

For instance $H = L^2(\Omega)$ and $f(u) = |u|^{p-1}u$, with $p > 1$.

Then, one needs to discover other properties of the underlying linear equation (smoothing, dispersion): IF $e^{At}u_0 \in X$, then look for solutions of the nonlinear problem in

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

One then needs to investigate whether

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

is locally Lipschitz. This requires extra work: We need to check the behavior of f in the space X. But the the class of functions to be tested is restricted to those belonging to X.
Typically in applications $X = L^r(0,T;L^q(\Omega))$. This allows enlarging the class of solvable nonlinear PDE in a significant way.

THE MORAL OF THIS STORY:

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!

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Consider the Linear Schrödinger Equation (LSE):

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

It may be written in the abstract form:

$$u_t = Au, \quad A = i\Delta = i\partial^2 \cdot /\partial x^2.$$

Accordingly, the LSE generates a group of isometries $e^{i\Delta t}$ in $L^2(\mathbf{R})$, i. e.

$$||u(t)||_{L^2(\mathbf{R})} = ||\varphi||_{L^2(\mathbf{R})}, \quad \forall t \geq 0.$$

The fundamental solution is explicit $G(x,t) = (4i\pi t)^{-1/2}\exp(-|x|^2/4i\pi t)$.

Dispersive properties: Fourier components with different wave numbers propagate with different velocities.

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

$$||u(t)||_{L^\infty(\mathbf{R})} \leq (4\pi t)^{-\frac{1}{2}} ||\varphi||_{L^1(\mathbf{R})}.$$

$$||u(t)||_{L^p(\mathbf{R})} \leq (4\pi t)^{-(\frac{1}{2}-\frac{1}{p})} ||\varphi||_{L^{p'}(\mathbf{R})}, \quad 2 \leq p \leq \infty.$$

- Local gain of $1/2$-derivative: If the initial datum φ is in $L^2(\mathbf{R})$, then $u(t)$ belongs to $H^{1/2}_{loc}(\mathbf{R})$ for a.e. $t \in \mathbf{R}$.

These properties are not only relevant for a better understanding of the dynamics of the linear system but also to derive well-posedness and compactness results for nonlinear Schrödinger equations (NLS).

The same L^2 theory applies for semilinear equations

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

provided the nonlinearity $f : \mathbf{R} \to \mathbf{R}$ is globally Lipschitz.

[Well-posedness of the linear problem + variation of constants formula]

BUT THIS ANALYSIS IS INSUFFICIENT TO DEAL WITH OTHER NONLINEARITIES, FOR INSTANCE:

$$f(u) = |u|^{p-1}u, \quad p > 1.$$

Despite of this, using the dispersive properties of the linear semigroup, the following can be proved for the NSE:

$$\begin{cases} iu_t + u_{xx} = |u|^p u & x \in \mathbf{R}, t > 0, \\ u(0,x) = \varphi(x) & x \in \mathbf{R}. \end{cases} \tag{2}$$

Theorem

(Global existence in L^2, Tsutsumi, 1987). For $0 \leq p < 4$ and $\varphi \in L^2(\mathbf{R})$, there exists a unique solution u in $C(\mathbf{R}, L^2(\mathbf{R})) \cap L^q_{loc}(L^{p+2})$ with $q = 4(p+1)/p$ that satisfies the L^2-norm conservation property and depends continuously on the initial condition in L^2.

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

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The three-point finite-difference scheme

Consider the finite difference approximation

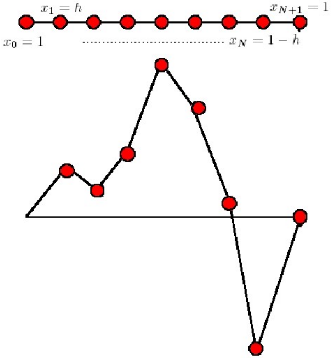
$$i\frac{du^h}{dt} + \Delta_h u^h = 0, t \neq 0, \quad u^h(0) = \varphi^h. \tag{3}$$

Here $u^h \equiv \{u_j^h\}_{j\in\mathbf{Z}}$, $u_j(t)$ being the approximation of the solution at the node $x_j = jh$, and $\Delta_h \sim \partial_x^2$:

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

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

In fact, $||u^h(t)||_{\ell^2} = ||\varphi||_{\ell^2}$, for all $t \geq 0$.



LACK OF DISPERSION OF THE NUMERICAL SCHEME

Consider the semi-discrete Fourier Transform

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

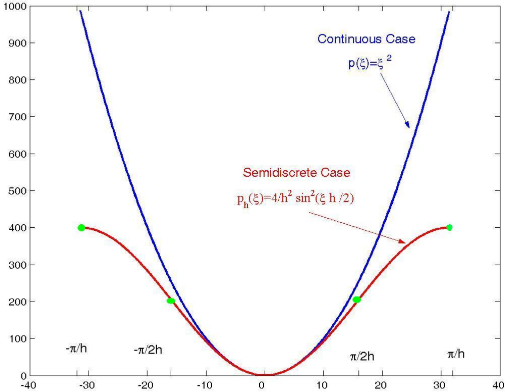
There are "slight" but important differences between the symbols of the operators Δ and Δ_h:

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

For a fixed frequency ξ, obviously, $p_h(\xi) \to p(\xi)$, as $h \to 0$. This confirms the convergence of the scheme. But this is far from being sufficient for our goals.

The main differences are:

- $p(\xi)$ is a convex function; $p_h(\xi)$ changes convexity at $\pm\frac{\pi}{2h}$.
- $p'(\xi)$ has a unique zero, $\xi = 0$; $p_h'(\xi)$ has the zeros at $\xi = \pm\frac{\pi}{h}$ as well.



LACK OF CONVEXITY = LACK OF INTEGRABILITY GAIN.

The symbol $p_h(\xi)$ looses convexity near $\pm\pi/2h$. Applying the stationary phase lemma (G. Gigante, F. Soria, IMRN, 2002):

Theorem

Let $1 \leq q_1 < q_2$. Then, for all positive t,

$$\sup_{h>0, \varphi^h \in l_h^{q_1}(\mathbf{Z})} \frac{|| \exp(it\Delta_h)\varphi^h ||_{l_h^{q_2}(\mathbf{Z})}}{||\varphi^h||_{l_h^{q_1}(\mathbf{Z})}} = \infty. \tag{4}$$

Initial datum with Fourier transform concentrated on $\pi/2h$.

LACK OF CONVEXITY = LACK OF LAPLACIAN.

Independent work on the Schrödinger equation in lattices:

- A. Stefanov & P. G. Kevrekidis, Nonlinearity 18 (2005) 1841-1857.
- L. Giannoulis, M. Herrmann & A. Mielke, Multiscale volume, 2006.

It is shown that the fundamental solution on the discrete lattice decays in L^∞ as $t^{-1/3}$ and not as $t^{-1/2}$ as in the continuous frame.

Lemma

(Van der Corput)
Suppose ϕ is a real-valued and smooth function in (a, b) that

$$|\phi^{(k)}(\xi)| \geq 1$$

for all $x \in (a, b)$. Then

$$\left| \int_a^b e^{it\phi(\xi)} d\xi \right| \leq c_k t^{-1/k} \tag{5}$$

LACK OF SLOPE= LACK OF LOCAL REGULARITY GAIN.

Theorem

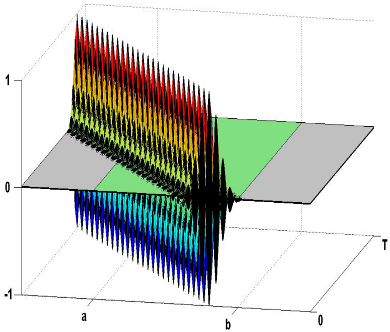
Let $q \in [1,2]$ *and* $s > 0$. *Then*

$$\sup_{h>0, \varphi^h \in l_h^q(\mathbf{Z})} \frac{\|S^h(t)\varphi^h\|_{\hbar^s_{loc}(\mathbf{Z})}}{\|\varphi^h\|_{l_h^q(\mathbf{Z})}} = \infty. \tag{6}$$

Initial data whose Fourier transform is concentrated around π/h.

LACK OF SLOPE= VANISHING GROUP VELOCITY.

Trefethen, L. N. (1982). SIAM Rev., **24** (2), pp. 113–136.



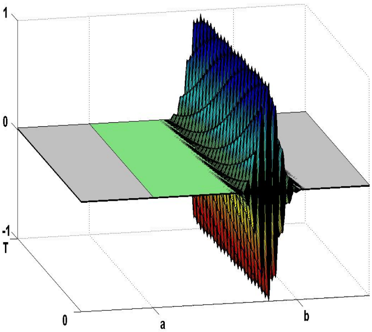


Figure: Localized waves travelling at velocity $= 1$ for the continuous equation (left) and wave packet travelling at very low group velocity for the FD scheme (right).

CONCLUSION

For the finite difference scheme:

- The standard L^2-stability condition does not suffice.
- We are dealing with properties that have to do with other integrability and regularity properties. Thus, stability has to be measured in those functional settings.
- Surprisingly enough the finite-difference scheme is not stable in that sense.

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A REMEDY: FOURIER FILTERING

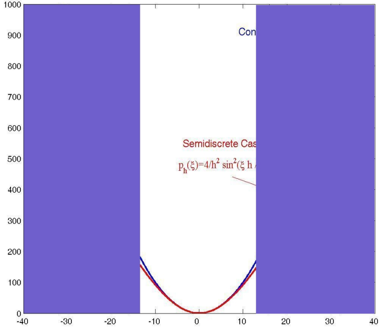
Eliminate the pathologies that are concentrated on the points $\pm\pi/2h$ and $\pm\pi/h$ of the spectrum, i. e. replace the complete solution

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

by the filtered one

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

This guarantees the same dispersion properties of the continuous Schrödinger equation to be uniformly (on h) true together with the convergence of the filtered numerical scheme.



But Fourier filtering:

- Is computationally expensive: Compute the complete solution in the numerical mesh, compute its Fourier transform, filter and the go back to the physical space by applying the inverse Fourier transform;
- Is of little use in nonlinear problems.

Other more efficient methods?

A VISCOUS FINITE-DIFFERENCE SCHEME

Consider:

$$\begin{cases} i\dfrac{du^h}{dt} + \Delta_h u^h = ia(h)\Delta_h u^h, & t > 0, \\ u^h(0) = \varphi^h, \end{cases} \tag{7}$$

where the numerical viscosity parameter $a(h) > 0$ is such that

$$a(h) \to 0$$

as $h \to 0$.

This condition guarantess the consistency with the LSE.

This scheme generates a *dissipative semigroup* $S_+^h(t)$, for $t > 0$:

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

Two dynamical systems are mixed in this scheme:

- the purely conservative one, $i\frac{du^h}{dt} + \Delta_h u^h = 0$,
- the heat equation $u_t^h - a(h)\Delta_h u^h = 0$ with viscosity $a(h)$.

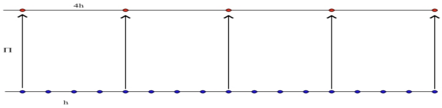
TWO-GRID ALGORITHM: DO NOT MODIFY THE SCHEME BUT SIMPLY PRECONDITION THE INITIAL DATA!

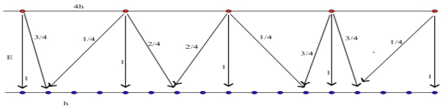
Let V_4^h be the space of slowly oscillating sequences (SOS) on the fine grid

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

where $E : \mathbf{C}_4^{h\mathbf{Z}} \to \mathbf{C}^{h\mathbf{Z}}$ stands for the extension operator and let $\Pi : \mathbf{C}^{h\mathbf{Z}} \to \mathbf{C}_4^{h\mathbf{Z}}$: be the projection operator

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



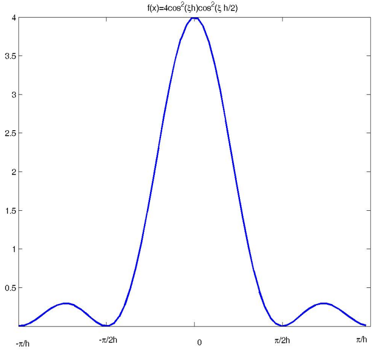


We now define the smoothing operator

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

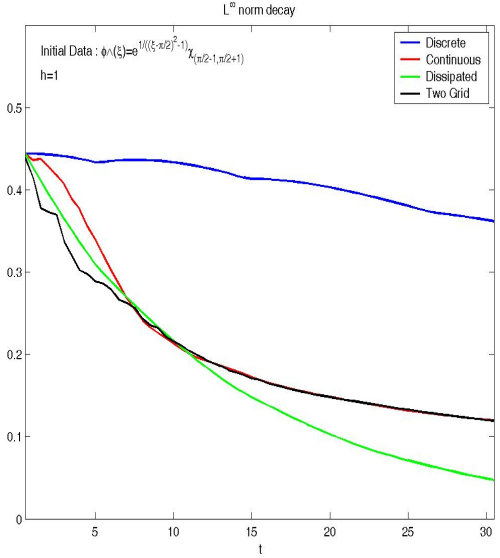
which acts as a a filter, associating to each sequence on the fine grid a slowly oscillating one. The discrete Fourier transform of a slowly oscillating sequence (SOS) is as follows:

$$\widehat{\widetilde{\Pi}\phi}(\xi) = 4\cos^2(\xi h)\cos^2(\xi h/2)\widehat{\Pi\phi}(\xi).$$



Both the viscous numerical scheme (with a correctly scaled viscosity coefficient) and the semi-discrete finite-difference scheme in the class of SOS data:

- Have the right decay and locally regularizing property.
- Provide efficient numerical schemes for the numerical approximation of the NLS and, in particular, to guarantee convergence in the context of the classical Tsutsumi's result mentioned above.


L^∞ norm decay
Initial Data : φ∧(ξ)=e^{1/((ξ-π/2)^2-1)} χ_(π/2-1,π/2+1)
h=1
Discrete
Continuous
Dissipated
Two Grid
0
0.1
0.2
0.3
0.4
0.5
5
10
15
20
25
30
t

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Is all this analysis needed?

In practice, we could:

- 1.- Approximate the L^2 initial data φ by smooth ones (say, in H^1)
- 2.- Use energy estimates in H^1, using Gronwall's inequality, since $f : H^1 \to H^1$ is now locally Lipschitz, to prove convergence of the scheme for these smooth data.
- 3.- By this double approximation procedure, derive a family of numerical solutions converging to the continuous one.

Note that:

- This can be done without using dispersive estimate.
- Warning! When doing that we pay a lot (!!!) at the level of the orders of convergence...

An example: The two-grid method yields the polynomial convergence rate:

$$||u^h - \mathcal{T}^h u||_{L^\infty(0,T;\ell^2(h\mathbf{Z}))} \leq C(T, ||\varphi||_{H^s}) h^{s/2}.$$

But, when applying the energy method for the finite-difference scheme we get a logarithmic order of convergence of $|\log h|^{-s/(1-s)}$ instead of $h^s/2$.

- Approximate φ by φ^ϵ smooth so that

$$||\varphi - \varphi^\epsilon||_{L^2} \sim \epsilon.$$

- Then

$$||\varphi^\epsilon||_{H^1} \sim \epsilon^{-s}.$$

- and

$$||u - u^\epsilon||_{L^2} \leq C\epsilon.$$

- Furthermore, by Gronwall, using H^1-estimates:

$$||u^\epsilon - u_h^\epsilon||_{L^2} \leq C \exp(C||\varphi^\epsilon||_{H^1}).$$

This, together with the following threshold in the aproximation process shows that the convergence is logarithmic without dispersive estaimates:

Lemma

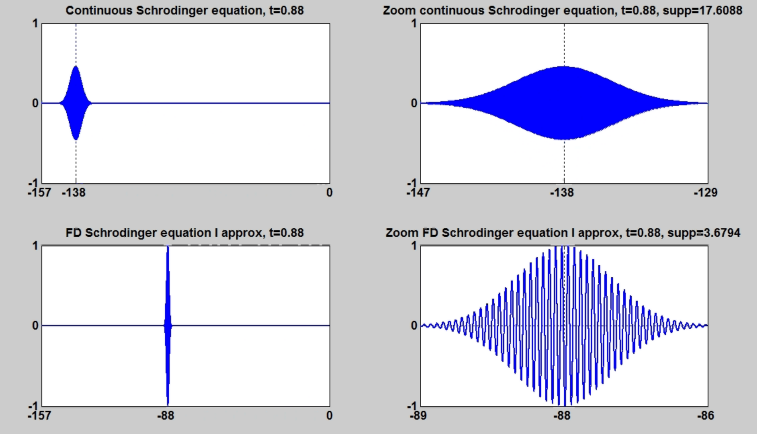
Let $0 < s < 1$ *and* $h \in (0,1)$. *Then for any* $\varphi \in H^s(\mathbf{R})$ *the functional* $J_{h,\varphi}$ *defined by*

$$J_{h,\varphi}(g) = \frac{1}{2}\|\varphi - g\|^2_{L^2(\mathbf{R})} + \frac{h}{2}\exp(\|g\|^2_{H^1(\mathbf{R})}) \tag{8}$$

satisfies:

$$\min_{g \in H^1(\mathbf{R})} J_{h,\varphi}(g) \leq C(\|\varphi\|_{H^s(\mathbf{R})}, s)|\log h|^{-s/(1-s)}. \tag{9}$$

Moreover, the above estimate is optimal.



Gaussian race: Continuous Schrödinger equation versus the finite-difference semi-discrete one. Initial datum: gaussian centered at $\pi/2$ in the Fourier variable.

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Conclusions

- Fourier filtering and some other variants (numerical viscosity, two-grid filtering,...) allow building efficient numerical schemes for linear and nonlinear Schrödinger equation: widder classes of nonlinearities, better convergence rates for rough data,...
- A systematic analysis of their computational efficiency is to be done.
- Much remains to be done to be develop a complete theory (multi-d, variable coefficients,...) and it should combine fine tools from harmonic analysis, PDE and Numerics.

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