Conservation of phase space properties for the cubic Schrödinger equation

Håvard Berland
Joint work with Alvaro Islas and Constance Schober

Department of Mathematical Sciences, NTNU, Norway
Department of Mathematics, University of Central Florida, USA

March 8, 2006 — MaGIC Ustaoset, Norway

Abstract

The cubic Schrödinger equation has an infinite number of known exact solutions through the Inverse Scattering Method. The nonlinear spectrum associated to the Lax pair of the equation reveals topological properties of the phase space solution that are difficult to assess by any other means. We use the invariance of the nonlinear spectrum of the associated Lax pair to examine the behaviour on a long time scale of exponential integrators and a multisymplectic integrator as compared with the split step approach, which is the most commonly used integrator for this particular problem. The initial condition used is a perturbation of the plane wave solution, which we know is unstable and thus presents a difficult task for numerical integrators. Our findings indicate that the exponential integrators from most viewpoints have a little edge over split step, while the multisymplectic, being almost as accurate, is too slow to compete.

(25 minute talk)

Overview

1. The cubic Schrödinger equation
2. Inverse scattering transform — Lax pair for CSE
3. Numerical instability
4. Nonlinear spectrum
5. Numerical results

Intent

Study how long numerical integrators can integrate an initial condition ϵ-close to an unstable solution.

The cubic Schrödinger equation

$$u_t = \mathrm{i} u_{xx} + 2\mathrm{i}|u|^2 u$$

We impose periodic boundary conditions, allows unstable solutions:

$$\psi(-2\sqrt{2}\pi, t) = \psi(2\sqrt{2}\pi, t), \quad t > 0.$$

Initial condition, perturbation of the (unstable) plane wave solution:

$$u(x,0) = \frac{1}{2}\left(1 + \epsilon \cos\left(\frac{x}{2\sqrt{2}}\right)\right)$$

In space, the equation is discretized spectrally. Thus, we only test performance of the time-integrator.

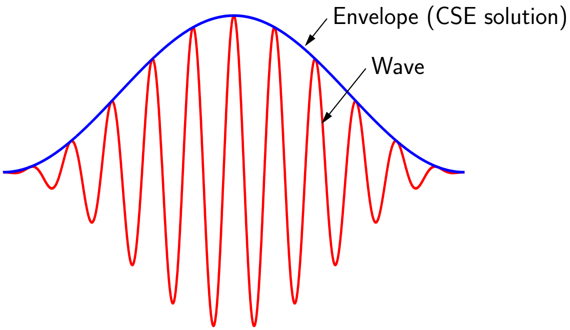
Physical significance of cubic Schrödinger

$$u_t = \mathrm{i}u_{xx} + 2\mathrm{i}|u|^2 u$$

- Its name is not due to relevance in quantum mechanics.
- Arises in nonlinear optics, deep water waves and plasma physics.
- The solution $u(x,t)$ describes in most contexts the space-time evolution of an envelope function of a fast oscillation.
- The most important physical properties of CSE:
  - Existence of soliton solutions.
  - Modulational instability for periodic boundary conditions.

Solitons

Solitons (in our context) are localized wave packets which survive collisions with one another. The solution $u(x, t)$ we obtain from integrating CSE are *envelopes* to the solitons.



In all plots, we visualize $|u|^2$, not the complex u.

The inverse scattering transform

- IST was initially used to show that the spectrum (scattering data, energy levels etc.) of the (linear) Schrödinger equation

$$\mathrm{i}\psi_t = -\psi_{xx} + U(x)\psi$$

  was invariant when the potential $U(x)$ is a solution of the KdV-equation $U_t + U_{xxx} + 6UU_x = 0$ [Gardner, Greene, Kruskal and Miura 1967].
- The basic principle is to transform time-evolution problem into a corresponding time-evolution problem on another set of data, the "scattering" data.
- Fourier transform can be seen as a special case of IST, with the Fourier coefficients as the scattering data.
- Zakharov and Shabat used the same methodology to prove existence of soliton solutions of the *cubic* Schrödinger equation [Zakharov and Shabat 1972].

Lax pair for cubic Schrödinger

The discovery of Zakharov and Shabat was the pair of operators

$$\mathcal{L} = \begin{pmatrix} \mathrm{i}\frac{\partial}{\partial x} & u^* \\ u & \mathrm{i}\frac{\partial}{\partial x} \end{pmatrix} \qquad \mathcal{A} = \begin{pmatrix} -\mathrm{i}|u|^2 & u_x^* \\ -u_x & \mathrm{i}|u|^2 \end{pmatrix}$$

- We will see that the spectrum $\sigma(\mathcal{L})$ is independent of time if *u is a solution of CSE*.
- Given the initial condition (and the initial spectrum), one can construct the physical solution at any given time using the inverse scattering transform at time t.
- This is done using Riemann θ-functions, and is possible "for all initial conditions of physical significance".
- All known conservation laws for the equation are linear combinations of the scattering data.

Invariance of spectrum

To see that the spectrum is invariant in time, ($\lambda_t = 0$) we compute

$$\frac{\partial}{\partial t}(\mathcal{L}\Psi) = \frac{\partial}{\partial t}(\lambda\Psi)$$
$$\mathcal{L}_t\Psi + \mathcal{L}\Psi_t = \lambda_t\Psi + \lambda\Psi_t \qquad (*)$$

We assume that the periodic function (in time) Ψ have the property

$$\Psi_t = \mathcal{A}\Psi.$$

By inserting this into (*) and rearranging we arrive at

$$(\mathcal{L}_t + [\mathcal{L}, \mathcal{A}])\Psi = \lambda_t\Psi$$

and thus $\mathcal{L}_t + [\mathcal{L}, \mathcal{A}] = 0$ is a condition on the Lax pair for invariance of the spectrum.

Invariance of spectrum, continued

By direct computation,

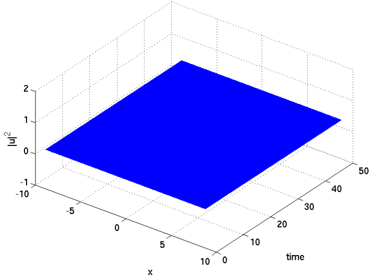
$$\mathcal{L}_t + [\mathcal{L}, \mathcal{A}] = \begin{pmatrix} 0 & u_t^* + \mathrm{i}u_{xx}^* + 2\mathrm{i}|u|^2 u^* \\ \mathrm{i}u_t + u_{xx} + 2|u|^2 u & 0 \end{pmatrix}$$

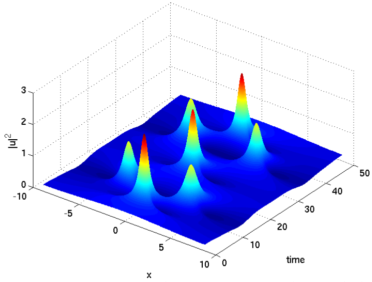
and we obtain the result

If u is a solution to the cubic Schrödinger equation then $\sigma(\mathcal{L})$ is invariant.

Instability

The initial condition we use is a perturbation of the *unstable* plane wave solution:

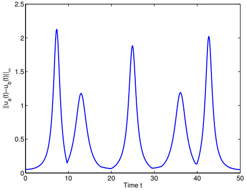




$u_a(x,0) = \frac{1}{2},\ u_a(x,t) = e^{it/2}/2$

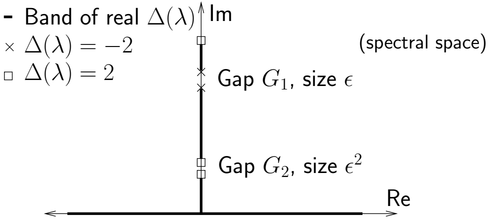
$u_b(x,0) = \frac{1}{2}\left(1 + \epsilon \cos\left(\frac{x}{2\sqrt{2}}\right)\right)$

Different perturbation parameters ϵ (0.1 used above) will lead to change in frequency for mode-excitation, but will not change magnitude $\|u_a(\cdot,t) - u_b(\cdot,t)\|_\infty$



Nonlinear spectrum of initial condition

The spectrum of $\mathcal{L}$ on our initial condition is computed numerically.

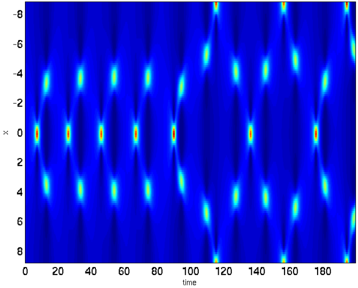


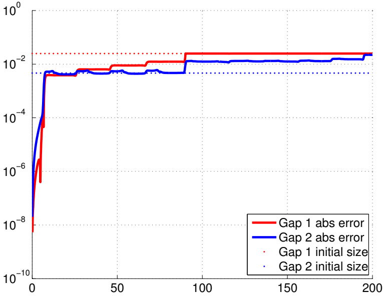
- The unstable plane wave solution has complex double points (unstable) where we now have gaps due to perturbation.
- Gaps in the spectrum correspond to the modes excited by the perturbation.
- We want to avoid *topological changes* in this spectrum.

Example with insufficient accuracy, homoclinic crossing

An example of an integration with insufficient accuracy. $N_{\mathcal{F}} = 128$, $h = 0.1$ and 'cfree4' as the integrator.

- Gap G_2 closes around $t = 7$ and G_1 closes at $t = 90$.
- Closure of biggest gap causes spatial dislocation of the center mode. Closure of smallest gap not easy to spot in the surface plot.

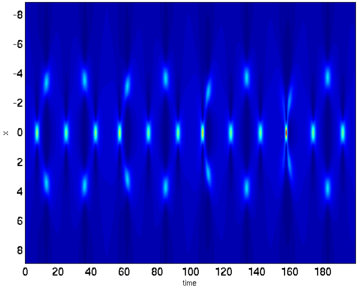


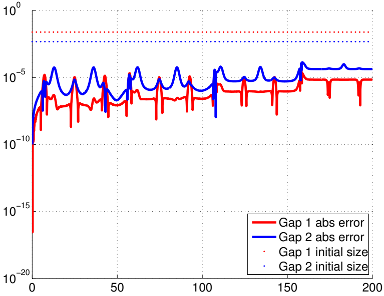


Example with sufficient accuracy

Increasing number of Fourier modes to 512 and using $h = 0.01$ we get a sufficiently accurate result

- No gap closures.
- Closure will happen in finite time, but is > 10000.
- Modes coalesce at around $t = 160$, even more challenging numerically





Integrators

- **cfree4** Exponential integrator of "ETD"-type, four stages, order 4, stiff order 2 [Celledoni, Martinsen, Owren 2003]
- **lawson4** Exponential integrator of Lawson-type, four stages, order 4, stiff order 1 [Lawson 1967]
- **splitstep4** Yoshida's coefficients are used to construct a fourth order scheme from the second order Strang splitting (same splitting as the exponential integrators use, linear part solved exactly, nonlinear part solved using RK4C).
- **msspectral** Second order, symplectic in time (implicit midpoint) and also in space (due to spectral discretization). Implicitness solved by simplified Newton iterations.

Numerical results, 64 and 128 Fourier modes

Time units before relative error of gap G_2 reaches 0.9. If it does, we assume it will soon close and solution can not be trusted from then on.

64 Fourier modes:

	$h = 10^{-1}$	$h = 10^{-2}$	$h = 10^{-3}$	$h = 10^{-4}$
cfree4	6.2	6.2	6.2	6.2
lawson4	n/a	6.2	6.2	6.2
splitstep4	n/a	6.2	6.2	6.2
msspectral	6.7	6.2	6.2	6.2

128 Fourier modes:

	$h = 10^{-1}$	$h = 10^{-2}$	$h = 10^{-3}$	$h = 10^{-4}$
cfree4	7.6	107.1	107.1	107.1
lawson4	8.4	107.1	107.1	107.1
splitstep4	n/a	107.1	107.1	107.1
msspectral	7.8	57.2	57.3	107.1

Numerical results, 256 and 512 Fourier modes

Time units before relative error of gap G_2 reaches 0.9. If it does, we assume it will soon close and solution can not be trusted from then on.

256 Fourier modes:

	$h = 10^{-1}$	$h = 10^{-2}$	$h = 10^{-3}$	$h = 10^{-4}$
cfree4	7.9	158	158	158
lawson4	11.4	158.1	158	158
splitstep4	n/a	2399	158	158
msspectral	7.9	207.6	158.1	158

512 Fourier modes:

	$h = 10^{-1}$	$h = 10^{-2}$	$h = 10^{-3}$	$h = 10^{-4}$
cfree4	7.8	> 10000	> 10000	
lawson4	n/a	5518	> 10000	
splitstep4	n/a	975	1596	
msspectral	5.9	109.8	> 500	

Computational cost

Number of integration steps per second, 2.4GHz Pentium IV

64 Fourier modes:

Integrator	$h = 0.1$	$h = 0.01$	$h = 0.001$
cfree4	1020	1090	1091
lawson4	913	1119	1114
splitstep4	424	435	444
msspectral	70	102	116

256 Fourier modes:

Integrator	$h = 0.1$	$h = 0.01$	$h = 0.001$
cfree4	594	649	657
lawson4	631	674.3	678
splitstep4	211	215	227
msspectral	2.6	4.3	5.1

Conclusions

- We did not find beneficial properties of the multisymplectic integrator weighing up for the increased cost.
- Cfree4 is in general a very good contender for solving the cubic Schrödinger equation numerically.
- Evaluation of the nonlinear spectrum is a precise way of determining numerical accuracy for long integration.

Results will be presented in a forthcoming paper,
H. Berland, A. Islas and C. Schober: *Conservation of phase space properties using exponential integrators on the cubic Schrödinger equation*.

References

- H. Berland, B. Skaflestad and W. Wright. Expint - A Matlab package for exponential integrators. 2005.
- A.L. Islas, D.A. Karpeev and C.M. Schober. Geometric integrators for the nonlinear Schrödinger equation. J. of Comp. Phys., 173:116–148, 2001
- A.L. Islas, and C.M. Schober. On the preservation of phase space structure under multisymplectic discretization. J. of Comp. Phys., 197:585–609, 2004.
- E.R. Tracy and H.H. Chen. Nonlinear self-modulation: an exactly solvable model. Phys. Rev. A (3), 37(3):815–839, 1988.