Numerical methods for the nonlinear Schrödinger equation

Master 2 – Modelling seminar

The nonlinear Schrödinger equation can be derived in many physical contexts, and in particular as enveloppe equations for the propagation of waves in various media. Its general form is

$$i\varepsilon\partial_t\psi(t,x) + \Delta\psi(t,x) = V(x)\psi(t,x) + f(|\psi(t,x)|)\psi(t,x),$$

where ψ is a complex-valued function that depends on time t and space $x \in \mathbb{R}^d$, and V and f are given functions.

For the physical applications it is often more important to preserve numerically some physical properties of the equations, such as time reversibility or mass conservation, than have high order approximations of the solutions. Therefore off-the-shelf generic are not a solution and specific methods have to be considered.

Having [1] as a starting point, we will investigate different methods: (Crank–Nicolson, relaxation, semi-implicit,...) finite difference methods, and pseudo-spectral methods. The goal is to understand the theoretical properties of these methods, and to illustrate these properties and understand the possible practical challenges of implementing them in 1 or 2D contexts.

Different further directions can be investigated, namely the comparison with generic methods, artificial boundary conditions, the addition of damping and angular rotation terms, or the behavior of these methods in the semi-classical regime (that is when ε is very small).

Background: numerical methods for ODE/PDE, Python programming.

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References

[1] Xavier Antoine, Weizhu Bao, and Christophe Besse. *Computational methods for the dynamics of the nonlinear Schrödinger/Gross–Pitaevskii equations.* Computer Physics Communications, **184**, 2621–2633 (2013). https://doi.org/10.1016/j.cpc.2013.07.012