A Wavelet-Galerkin method for the nonlinear Schrödinger equation.

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December 24, 2021

Abstract

A general implementation is presented for constructing a wavelet method for solving the nonlinear equation of Schrödinger. An explicit formula is derived which yields a stability in of the numerical solution. A simulation is elaborated to show the general behavior of the distribution function. Numerical results and comparison with classical algorithms are provided. This approach prove an attractive scheme for solving such equation.

1 Introduction

The general one dimensional Schrödinger equation is given as follows:

$$\hat{H}\psi(x,t) = E\psi(x,t)$$

Where $\hat{H}$ is the Hamiltonian operator, ψ is the wave function, and E is the energy. In atomic units, the Hamiltonian operator for a particle in a potential is:

$$\hat{H} = - \bigtriangledown^2 + V(x)$$

The time-independent Schrödinger equation (TISE) bounded inside a potential becomes:

$$\psi_x x(x,0) + V(x)\psi(x,0) = E\psi_t(x,0)$$

(ψ is the time-independent wave function) For a particle in a time-dependent potential, the one-dimensional Schrödinger equation is

$$\frac{-h^2}{2m}\psi_x x(x,t) + V(x)\psi(x,t) = E\psi_t(x,t)$$

where m is the mass of the particle, $V(x)$ is the potential that the particle moves in, and $\psi(x,t)$ is the particle's wave function. The physical interpretation of the wave function is that $\psi^*(x,t)\psi(x,t)dx$ is the probability of finding the particle between x and $x + \Delta x$. The notation ψ^* denotes taking the complex conjugate. In general the wave function $\psi(x,t)$ will be complex, not real.

For bound state problems we generally require that the wave function be normalized, which is to say that $\int \psi^*(x,t)\psi(x,t)dx = 1$ where the integral runs over all possible values

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of x. This condition simply means that if we look everywhere, we find the particle once and only once.

In quantum mechanics a particle does not have a definite position (at least not until we measure the particles position) but only has a probability of being found at a position. If we have a million hydrogen atoms all in the ground state and we measure the position of the electron in all million atoms, we will get a different answer for each atom. It does not make sense to talk about a definite position in a quantum system but only an average position. Since $\psi^*(x,t)\psi(x,t)$ is the probability distribution, the average position of a particle is $< x >= \int \psi^*(x,t)\psi(x,t)dx$. In quantum mechanics angular brackets are used to denote an average. In general, the average or expectation value of an observable O is $< O >= \int \psi^* O\psi dx$ and order matters! You cannot interchange the O and ψ^* or ψ except in special cases.

Numerical solution of the Schrödinger's equation have been proposed by many authors. Some results are obtained by using collocation scheme [13-14]. Arico and Co [5] set upinverse scattering transform incorporating characteristics with which to obtain a numerical solution via a weighted residual method. Weidman [18] have discussed the comparison of a number of different numerical approaches to the equation. The wavelets approach is discussed by Ahsan and Co [3]. Many other authors [2],[17] have used a variety of numerical techniques based on finite-difference and finite-element methods in attempting to solve the equation.

We propose the use of the Galerkin-Wavelets scheme for solving the Schrödinger's equation which use multi-resolution analysis of all possible candidate stencils to construct the solution.

2 Algorithm of Standard Galerkin

The formulation of the algorithm of Galerkin from just the following series of spaces V_j of a multi-resolution analysis is presented as follows:

To find $u_p(x,t) = \sum_{k=0}^{2^p-1} C_{pk}(t)\phi_{pk}(x)$ where

$$\forall k, \qquad \frac{\partial}{\partial t}C_{pk}(t) + \sum_l C_{pk} < u^* \frac{\partial \phi_{pl}}{\partial x}, \phi_{pk} >= -\nu \sum_l C_{pl} < \frac{\partial \phi_{pl}}{\partial x}, \frac{\partial \phi_{pk}}{\partial x} > \tag{2.1}$$

where $< ., . >$ stands for the $L^2(\mathbb{R})$ inner product.

If $C_p = (C_{pk})_{k=0,2^p-1}$ then

$$\frac{\partial}{\partial t}C_p(t) + AC_p(t) = 0 \tag{2.2}$$

where A is a matrix with the general term

$$A_{kl} =< u^* \frac{\partial \phi_{pl}}{\partial x}, \phi_{pk} > -\nu \sum_l C_{pl} < \frac{\partial \phi_{pl}}{\partial x}, \frac{\partial \phi_{pk}}{\partial x} >$$

Many solutions are enabled to integrate those differential equation (system):

1. Direct integration while using e^{-tA}.
2. Numerical integration after discretization by finite difference.

In this second case we use often some implicit schemes for the term of diffusion (elliptical) and we will be therefore leaded to inverse an ill conditioned matrix. It is useful to use in the place of the basis of $(\phi_{pk})_{0\leq k\leq 2^p-1}$ those of $(\psi_{jk})_{0\leq j\leq p-1}^{0\leq k\leq 2^j-1}$, to reformulate and preconditioning the problem with the diagonal matrix of the operator Γ^2: $\psi_{jk}\mapsto 2^j\psi_{jk}$.

The formulation of Galerkin use a particular approximation of the operator of evolution $u^*\frac{\partial}{\partial x}-\nu\frac{\partial^2}{\partial x^2}$. It is not very well adapted in case that the space of the approximation space is adapted to the solution because in this case it's necessary to recalculate all the matrix (or at least a part).

3 Wavelet-Galerkin method

We write a weak formulation while using one family of functions $(\theta_\lambda(x))$:

$$\frac{\partial}{\partial t}<u,\theta_\lambda>+\frac{1}{2}<\frac{\partial u}{\partial x}u^*,\theta_\lambda>-\nu<\frac{\partial^2 u}{\partial x^2},\theta_\lambda>=0 \tag{3.3}$$

and we discretize directly in time for example by an implicit Euler's scheme for the term of diffusion and explicit for the term $u^*\frac{\partial u}{\partial x}$.
If $(<u^n,\theta_\lambda>)$ are the news unknowns we have:

$$\frac{<u^{n+1},\theta_\lambda>-<u^n,\theta_\lambda>}{\Delta t}+<\frac{1}{2}\frac{\partial u}{\partial x}u^*,\theta_\lambda>-\nu<\frac{\partial^2 u}{\partial x^2},\theta_\lambda>=0 \tag{3.4}$$

that we write

$$<(I-\Delta t\nu\frac{\partial^2}{\partial x^2})u^{n+1},\theta_\lambda>=-\Delta t<(\frac{1}{2}\frac{\partial u}{\partial x}u^*)^n,\theta_\lambda>+<u^n,\theta_\lambda>=0. \tag{3.5}$$

We will choose now θ_λ such that $<(I-\Delta t\nu\frac{\partial^2}{\partial x^2}),\theta_\lambda>=\psi_\lambda$ where ψ_λ is a family of r-regular wavelets $(r\geq 2)$), then

$$<u^{n+1},\psi_\lambda>=-\Delta t<(\frac{1}{2}\frac{\partial u}{\partial x}u^*),\theta_\lambda>+<u^n,\theta_\lambda>, \tag{3.6}$$

and

$$u^{n+1}=\sum_\lambda(-\Delta t<(\frac{1}{2}\frac{\partial u}{\partial x}u^*),\theta_\lambda>+<u^n,\theta_\lambda>)\psi_\lambda. \tag{3.7}$$

u^{n+1} is the exact solution of the discretized problem in time and λ describe a family of indices Λ_V then $u^{n+1}=\sum_\lambda(u^n-\Delta t<(\frac{1}{2}\frac{\partial u}{\partial x}u^*),\theta_\lambda>+<u^n,\theta_\lambda>)\psi_\lambda$ is the orthogonal propagation of u^{n+1} in V.

We know that some rapid algorithms of reconstruction allow to get u_V^{n+1} from its wavelets coefficients $(u^n-\Delta t<(\frac{1}{2}\frac{\partial u}{\partial x}u^*),\theta_\lambda>)$.
The computation of these scalar products can be speedily done, indeed θ_λ follows ψ_λ. Then, For all ϵ, there exist one constant n_ϵ such that, for all function f,

$$|<f-\pi_{V_{j+n_\epsilon}}f,\theta_{jk}>|\leq C(f)\epsilon. \tag{3.8}$$

Algorithm	$2\pi\ T_{max}$	$S_{max}/2$		dimension
$V^{(n)} = V_8$	1.64	150.3	no oscillations	256
$V^{(n)} = V_7$	1.63	135.0	localized oscillations	128
$V^{(n)}$ adapted	1.64	150.3	no oscillations	≤ 104
Fourier pseudospectral $n = 128$	1.62	134.8	spread oscillations	128

Table 1: Comparison of some different methods

n_ϵ is independent of j which for a given ϵ, some rapid algorithms (in tree) can be used to compute the scalar product $< f, \theta_{jk} >$.

This approach leads to some rapid and adaptative algorithms. The obtained numerical results compare favorably to those obtained by classical approaches in term of precision and cost (see Table 1).

The computation of some nonlinear terms in the initial equation (u^2) is a real difficulty in the case of adaptative spaces. Indeed, in this case, the collocation approaches are difficult even though there are the most efficient in the case of regular spaces (V_j) holding interpolative functions.

Starting from the discretized equation in time and for $\theta_\lambda = \psi_\lambda$ we write

$$< (I - \Delta t\nu \frac{\partial^2}{\partial x^2})u^{n+1}, \psi_\lambda >= -\Delta t < \frac{1}{2}\frac{\partial (u^* u)^n}{\partial x}, \psi_\lambda > + < u^n, \psi_\lambda >= 0, \tag{3.9}$$

and if we define $(I - \Delta t\nu \frac{\partial^2}{\partial x^2})\psi_\lambda = \theta'_\lambda$, we have:

$$< u^{n+1}, \theta'_\lambda >= -\Delta t < (\frac{1}{2}\frac{\partial uu^*}{\partial x}), \psi_\lambda > + < u^n, \psi_\lambda > \tag{3.10}$$

θ'_λ and θ_λ are two bi-orthogonal families and $\Pi_\Lambda u^{n+1} = \sum_{\lambda\in\Lambda} < u^{n+1}, \theta'_\lambda > \theta_\lambda$.

As compared to the first approach, the difficulty is not to compute the scalar product $< u^{n+1}, \theta_\lambda >$ since it is the wavelets coefficients of $u^n - \frac{\Delta t}{2}\frac{\partial}{\partial x}(uu^*)$ but to "rebuild" $\Pi_\Lambda u^{n+1}$ from the sum $\sum < u^{n+1}, \theta'_\lambda > \theta_\lambda$.
Rapid algorithms are still available and inspired from those defined for homogeneous operators and the associated bi-orthogonal multi-resolutions analysis .

For a bounded Lipschitzienne real function $a(x)$, consider the problem:

$$\begin{cases} (I - \frac{\partial}{\partial x}(a(x)\frac{\partial}{\partial x}))u = f \\ u(0) = u(1). \end{cases} \tag{3.11}$$

The localization of the wavelets ψ_{jk} for big j, allows us to think that in order to such values of j, the operator $(-a(k2^{-j}\frac{\partial^2}{\partial x^2})$ is close to the operator L^{-1} when we apply it to the wavelets ψ_{jk}. This is not realistic only for big j and, for the smooth part of the problem it's necessary to use a more classical approach.
In fact, we build an approximation of L^{-1} from the following theorem:

Theorem 1 *: Consider A_q the approximation of Galerkin of L^{-1} in V_q by:*

$$A_q = \Pi_q^*(\Pi_q L \Pi_q^*)\Pi_q$$

where Π_q termed the projection in V_q and Π_q^* the extension of V_q in L^2.
Define P_q the operator as:

$$\psi_{jk} \mapsto P_q(\psi_{jk}) = \theta_{jk}, \qquad where\ -a(k2^{-j})\frac{\partial^2}{\partial x^2}\theta_{jk} = \psi_{jk},\ \forall j \geq q$$

$$P_q = 0\ on\ V_q$$

so if $L(A_q + P_q) = I - u$, there exists a constant C dependent of $a(x)$ and of the multi-resolutions analysis such that $\|u^2\|_{L^2,L^2} \leq C2^{-q}$. We get then $P(u) \leq C2^{-q/2}$ and the Neumann's serie $\sum_{k=0}^{\infty} u^k$ converge, it means that $L^{-1} = (A_q + P_q)\sum_{k=1}^{\infty} u^k$.

A numerical algorithm is then possible and provides an approximation of L in V_p from the approximation of Galerkin of f in V_q $(q < p)$ and the diagonal operator of constant coefficients in the basis some $(\psi_{jk})_{j\geq q, j\leq p-1}$.

4 Application on Schrödinger's equation

We explore simulating the 1-dimensional time-dependent Schrödinger equation (TDSE). Assuming $h = 1$, the equation is

$$\frac{\partial}{\partial t}\Psi(x,t) = -i\hat{H}\Psi(x,t)$$

where $\hat{H}$ is the Hamiltonian operator) and $\Psi(x,t)$ is the wave function of the quantum system. If the Hamiltonian is independent of time, then the equation can be written in terms of a time evolution operator,

$$\Psi(x,t) = e^{-i\hat{H}t}\Psi(x,0)$$

For a single non-relativistic spinless particle of mass, $m = 1$, in a time-invariant potential, $V(x)$, the Hamiltonian is given by

$$\hat{H} = -\frac{1}{2}\nabla^2 + V(x)$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2}$ is the Laplace operator.

We use a localized Gaussian wave centered at x_0 with average initial momentum, p_0 , and Gaussian width, σ_0 . The wave function is given by

$$\psi(x) = \left(\frac{1}{2\pi{\sigma_0}^2}\right)^{\frac{1}{4}} \exp\left(-\frac{(x-x_0)^2}{4{\sigma_0}^2} + ip_0x\right)$$

As a free particle, the Gaussian wave packet's center moves by p_0t over time t (since we set the mass to 1 earlier, the momentum is equal to the velocity). The uncertainties in position and momentum are given by $\Delta x = \sigma_0$ and $\Delta p = (2\sigma_0)^{-1}$, respectively. The Gaussian wave packet is a minimum uncertainty wave packet with $\Delta x \Delta p = 1/2$. Consistent with the motion of a free particle, Δp is constant in time.

The energy of the particle is $E = p_0^2/2$.

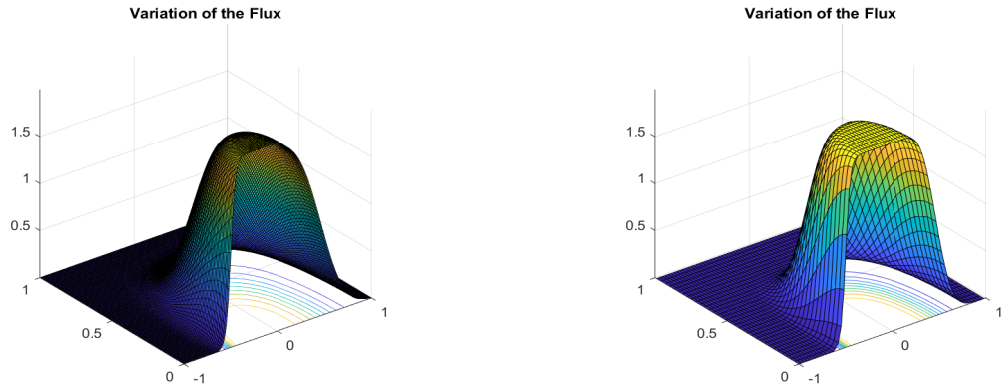

Figure 1: Time evolution of the numerical solution

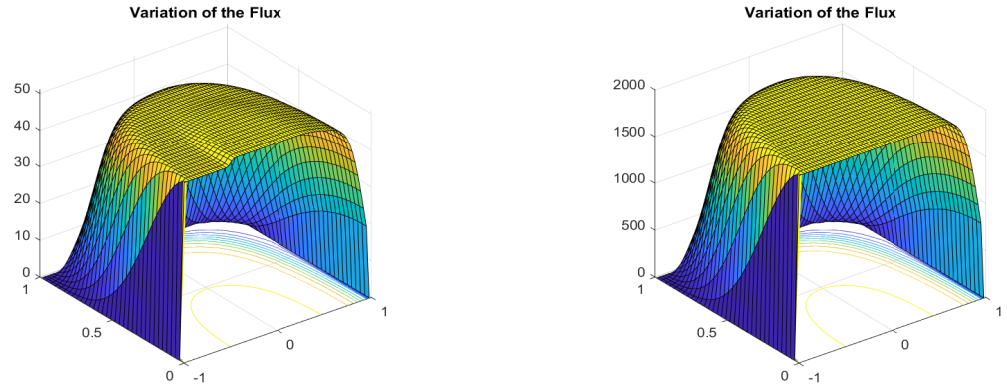

Figure 2: Schrödinger's equation solution at various times.

5 Conclusion

The numerical resolution of Schrödinger's equation has been performed using wavelet scheme. This method is based on the wavelet representation of the space of the approximation. Comparison with other classical algorithms is given and shows the efficiency of our method.

We have demonstrated that the wavelets methods can be naturally applied to integrate the nonlinear Schrödinger equation. We have shown that a simple spatial discretization leads to a Hamiltonian system, whose solution has been proved to converge to the solution when the spatial stepsize goes to zero. The accuracy and the conservation properties of the integrators have been examined numerically. In particular, it has been shown that the wavelets approach are able to preserve rather well the invariants of the equation, such as charge, energy, and momentum. The convergence of the formal energy has been checked to be in good agreement with the conjecture.

Extensions to realistic problems with different boundary conditions and multidimension are our future research.

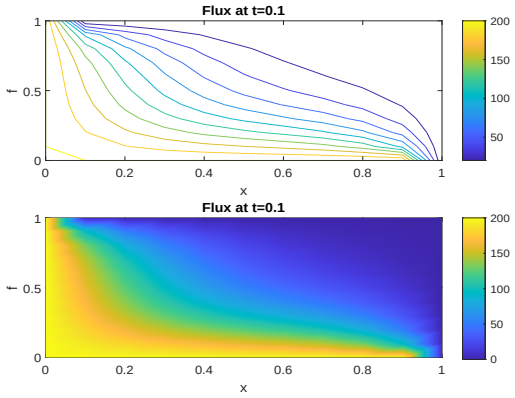

Figure 3: Flux behavior.

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