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Simulation Electromagnetic Waves Throughtime-Dependent Schrödinger Equation Using WENO Schemes

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ABSTRACT

We present a numerical simulation forSchrödinger equation. It is based on the weighted essentially non-oscillatory(WENO). To obtain finite-dimensional subspaces we first discuss semi-discretization with respect to the scale parameter by means of sparse grids which relies on mixed regularity and decay properties of the wave functions. We then apply the new schemes to evaluate the density and the total energy of the distribution function. The results are compared to classic numerical methods and give a general view on the reducing of the relative errors. with consistency.

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INTRODUCTION

The nonlinear Schrödinger equation (NLS) equation is very important in Mathematics, as well as in Physics and Engineering, as it arises in modeling electromagnetic waves in optical fibers (Zakharov, V.E. and A.B. Shabat, 1971) and surface waves in deep waters.
In the focusing case the NLS equation is

$$-\frac{h^2}{2m}\Psi_{xx}(x,t)+V(x)\Psi(x,t)=E\Psi_t(x,t). \quad (1)$$

When the initial potential$\Psi(x,t)$ is given,which represents the case that is of most interest in applications, one has tosolve the initial value problem (IVP) for (1).

Such a problem belongs to the class of "integrable nonlinear equations", whichmeans that it is solvable by theinverse scattering transform(IST) method (Novikov, S., 1984; Hu, C.Q., C.W. Shu, 1999; Ablowitz, M.J. and P.A. Clarkson, 1991). In spite of this fact, the earlier methods but one (Arico, A., 2009) do not make use ofthe IST method for obtaining a numerical approximation of the exact solutionof the IVP for (1). In fact, the numerical method most used is the split stepFourier method introduced by Lake *et al*. and by Hardin and Tappert. Taha and Ablowitz (1984) made a comparative analysis of numerical methods to solve the IVP for (1), such as various finite-difference schemes (e.g., theAblowitz-Ladik scheme (1991), split-step Fourier methods and pseudo-spectral methods (Fornberg, B., 1996; Fornberg, B. and G.B. Whitham, 1978) and decided in favour of the split-step Fourier method with spectral methods as a second choice.

The dominant numerical method became the split-step Fourier (SSF) method(e.g., (Weideman, J.A.C. and B.M. Herbst, 1986)) even though in the 1990' orthogonal splines methods were successfully applied to solve the IVP for (1) (Robinson, M.P., 1997; Liu, X.D., 1994; Robinson, M.P., 1993).

In order to illustrate our contribution, let us first recall that, as found invarious sources (e.g., (Zakharov, V.E. and A.B. Shabat, 1971; Ablowitz, M.J. and P.A. Clarkson, 1991; Ablowitz, M.J., 2004; Novikov, S., 1984)), the solution of the IVP for (1) by theIST method is composed of the following three steps:
(1) solve the direct scattering problem for the associated Zakharov-Shabat (ZS) system to obtain thescattering data;
(2) propagate the initial scattering data in time;
(3) solve theassociated inverse scattering problem, to arrive to the solution we are lookingfor.

Our numerical method solves the problem, allowing oneto obtain a very good approximation of$\Psi(x,t)$.

In the following sections we introduce the one dimensional Schrodinger equation with time dependence, then defining the discrete wavelets transforms and the ameliorate one the fast wavelets transform. At the end we present a numericalsimulation for the resolution of the main problem.

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Schrödinger's Equation:

The general one dimensional Schrödinger equation is given as follows:

$$\widehat{H}\Psi(x,t) = E\Psi(x,t) \quad (2)$$

Where Ĥ 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:

$$\widehat{H} = -\nabla^2 + V(x)$$

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

$$-\Psi_{xx}(x,0) + V(x)\Psi(x,0) = E\Psi_t(x,0) \quad (3)$$

(Ψis the time-independent wave function)

For a particle in a time-dependent potential, the one-dimensional Schrödinger equation is

$$-\frac{h^2}{2m}\Psi_{xx}(x,t) + V(x)\Psi(x,t) = E\Psi_t(x,t) \quad (4)$$

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 notationΨ^* 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 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 milΨlion 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 $\mathcal{O}$ is $< O >= \int \Psi^* \mathcal{O} \Psi dx$and order matters! You cannot interchange the $\mathcal{O}$andΨ^* or Ψ except in special cases.

WENO Schemes:

The basic idea of WENO, which is based on ENO of course, is the following: instead of using only one of the candidate stencils to form the reconstruction, one uses a convex combination of all of them. So suppose the k candidate stencils

$$S_r(i) = x_{ir},..., x_{ir+k}, \qquad r = 0,..., k-1 \quad (2.5)$$

produce k different reconstructions to the value $v_{i+1/2}$, according to (20),

$$v_{i+\frac{1}{2}}^{(r)} = \sum_{j=0}^{k-1} c_{rj}\bar{v}_{i-r+j}, \qquad r = 0,\ldots,k-1 \quad (2.6)$$

WENO reconstruction would take a convex combination of all $v_{i+1/2}^{(r)}$ defined in (53) as a new approximation to the cell boundary value $v(x_{i+1/2})$:

$$v_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} w_r v_{i+1/2}^{(r)}, \quad (2.7)$$

We require

$$w_r \geq 0, \qquad \sum_{j=0}^{k-1} w_r = 1 \quad (2.8)$$

for stability and consistency.

If the function *v*(*x*) is smooth in all of the candidate stencils (52), there are constants d_r such that

$$v_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} d_r v_{i+1/2}^{(r)} = v(x_{i+1/2}) + o(\Delta x^{2k-1}), \quad (2.9)$$

and for the other

$$v_{i-\frac{1}{2}} = \sum_{j=0}^{k-1} \tilde{d}_r v_{i+1/2}^{(r)} = v(x_{i-1/2}) + o(\Delta x^{2k-1}), \quad (2.10)$$

we have by symmetry

$$\tilde{d}_r = d_{k-1-r} \tag{2.11}$$

For example, d_r for $1 \le k \le 3$ are given by

$$d_0 = 1, \quad k = 1;$$
$$d_0 = \frac{2}{3}, \quad d_1 = \frac{1}{3}, \quad k = 2$$
$$d_0 = \frac{3}{10}, \quad d_1 = \frac{3}{5}, \quad d_2 = \frac{1}{10}, \quad k = 3$$

we can see that d_r is always positive and, due to constency,

$$\sum_{r=0}^{k-1} d_r = 1$$

The weights should be smooth functions of the all averages involved. In fact, the weights described below are*C1*. We would like to have weights which are computationally efficient. Thus, polynomials or rational functions are preferred over exponential type functions.

All the considerations lead to the following form of weights:

$$w_r = \frac{\alpha_r}{\sum_{s=0}^{k-1} \alpha_s}, \qquad r = 0,..., k-1 \tag{2.12}$$

with

$$\alpha_r = \frac{d_r}{(\varepsilon + \beta_r)^2} \tag{2.13}$$

Here $\varepsilon > 0$ is introduced to avoid the denominator to become 0 and β_r is a smoothness measurement of

Consideration for a smooth flux and for the role of higher order variations leads us to the following measurement for the smoothness: let the reconstruction polynomial on the stencil $S_r(i)$ be denoted by $p_r(x)$, we define*:*

$$\beta_r = \sum_{l=0}^{k-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \Delta x^{2l-1} \left(\frac{\partial^l p_r(x)}{\partial^l x} \right) dx. \tag{2.14}$$

The right hand side is just a sum of the squares of scaled L^2 norms for all the derivatives of the interpolation polynomial $p_r(x)$ over the interval $(x_{i-1/2}, x_{i+1/2})$. The factor Δx^{2l-1} is introduced to remove any Δx dependency in the derivatives.

For example, when *k* = 2

$$\begin{cases} \beta_0 = (\bar{v}_{i+1} - \bar{v}_i)^2, \\ \beta_1 = (\bar{v}_i - \bar{v}_{i-1})^2. \end{cases} \tag{2.15}$$

and for *k* = 3, (61) gives:

$$\begin{cases} \beta_0 = \frac{13}{12}(\bar{v}_i - 2\bar{v}_{i+1} - \bar{v}_{i+2})^2 + \frac{1}{4}(3\bar{v}_i - 4\bar{v}_{i+1} - \bar{v}_{i+2})^2, \\ \beta_1 = \frac{13}{12}(\bar{v}_{i-1} - 2\bar{v}_i - \bar{v}_{i+1})^2 + \frac{1}{4}(\bar{v}_{i-1} - \bar{v}_{i+1})^2, \\ \beta_2 = \frac{13}{12}(\bar{v}_{i-2} - 2\bar{v}_{i-1} + \bar{v}_i)^2 + \frac{1}{4}(\bar{v}_{i-2} - 4\bar{v}_{i-1} + 3\bar{v}_i)^2 \end{cases} \tag{2.16}$$

Now, we can form the weights w_r and $\overline{w}_r$ using (59)-(60)

and

$$\tilde{w}_r = \frac{\alpha_r}{\sum_{s=0}^{k-1} \tilde{\alpha}_s}, \qquad \tilde{\alpha}_r = \frac{\tilde{d}_r}{(\varepsilon + \beta_r)^2}. \tag{2.17}$$

Finaly, we can find the (2*k*-1)-th order reconstruction

$$v^{+}_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} w_r v^{(r)}_{i+1/2}$$
$$v^{-}_{i-\frac{1}{2}} = \sum_{j=0}^{k-1} \tilde{w}_r v^{(r)}_{i-1/2} \quad (2.18)$$

And now, we can return to the monotone flux choosed before for the ENO schemes then follows all the steps as in it (use (48) to compute the flux then form the scheme (6)).

RESULTS AND DISCUSSION

So far we have looked at states that were either energy eigenstates or a superposition of a small number of energy eigenstates. However for some problems, such as scattering problems, we want solutions that are not energy eigenstates but are solutions to the full time-dependent Schrödinger equation.

$$-\frac{h^2}{2m}\Psi_{xx}(x,t) + V(x)\Psi(x,t) = E\Psi_t(x,t) \quad (38)$$

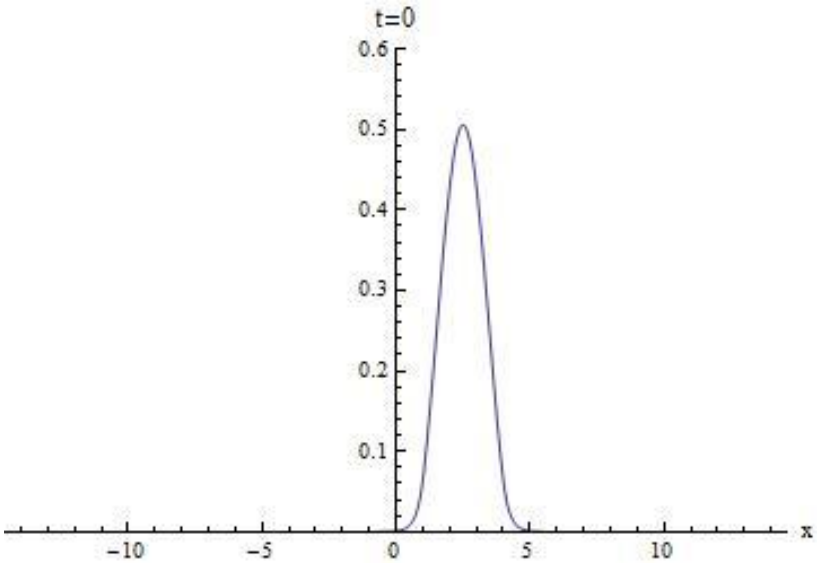
Suppose for the moment that we have a free particle so that V(x,t)=0. The time dependent Schrödinger equation is then

$$-\frac{h^2}{2m}\Psi_{xx}(x,t) = E\Psi_t(x,t) \quad (39)$$

and has solutions of the form $\Psi(x,t) = Ae^{i(kx-\omega t)}$ which gives $\frac{h}{2m}k^2 = \omega$ a dispersion relation relating the wave number *k* to the angular frequency ω. Remember that the wave number is related to the wavelength by $k = \frac{2\pi}{\lambda}$ and that the momentum of a particle is *p=h k*. The Schrödinger equation is linear so a sum of solutions is also a solution. Thus a wave function of the form

$$\Psi(x,t) = \sum_i Ae^{i(k_i x-\omega_i t)} \quad (40)$$

is also a solution. In equation (40) the sum runs over the allowed wave numbers k_i. If we have just one wave number, the particle has a definite momentum but is not spatially localized. This is easily seen by computing $P(x,t) = \Psi^*(x,t)\Psi(x,t)$ which is a constant if $\Psi(x,t) = Ae^{i(kx-\omega t)}$ indicating that the particle has an equal probability of being found anywhere in space. This is consistent with the uncertainly principle, since $\Delta p = 0$ we must have $\Delta x = \infty$. The situation is different if we have a state with many wave numbers. Suppose we have a state with 101 different wave numbers. The wave numbers are Gaussian distributed around 5. The units are chosen so that *h=1*and the particle has unit mass.



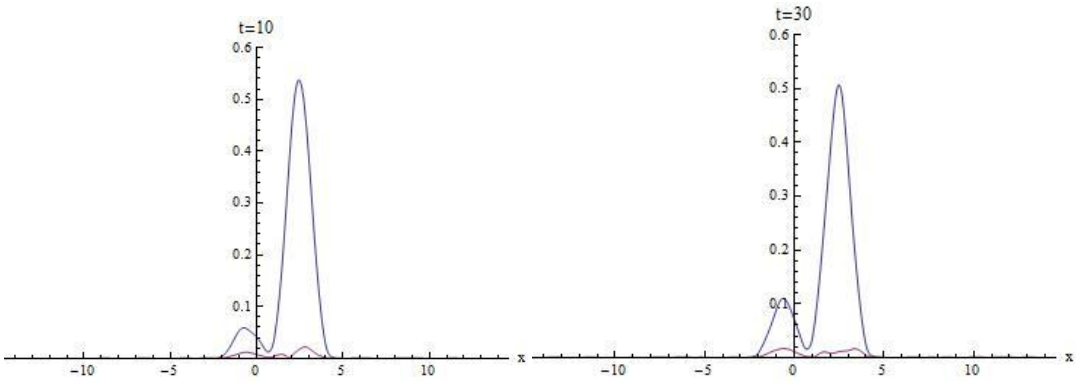


Fig. 1: The probability density with energy shows that our state is localized in space and is right moving.

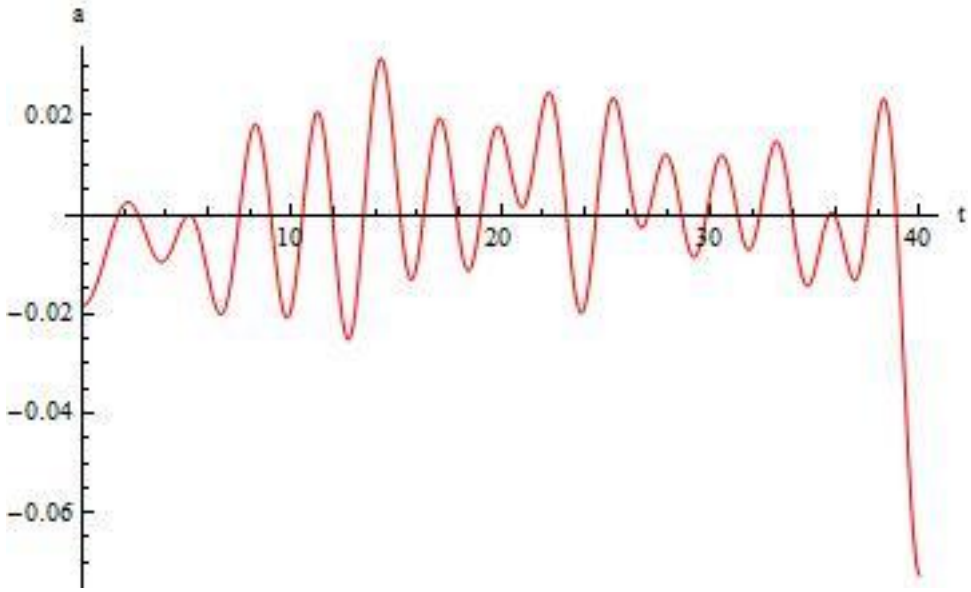


Fig. 2: Evolution of the errors in the distribution function.

Conclusion:

In this article we proposed to use a WENO scheme to find the numerical solution of the time-dependent Schrödinger equation. The sparse grid constructions promises to break the curse of dimensionality to some extent and may allow a numerical treatment of the Schrödinger equation without resorting to any model approximation. Furthermore we studied a discretization with respect to the level and introduced generalized discrete sparse grid spaces. Using this new non oscillatory scheme for the evaluation of the distribution function along time in the stable position, we control the error along the time with the conservation of the properties of the electromagnetic waves. The numerical simulation shows that this method gives a well approximated solution for the time dependent Schrödinger equation. We look forward to extend this scheme to the two dimensional case.

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