A STUDY OF THE FINITE DIFFERENCE METHODS AND THE WENO SCHEMES IN THE RESOLUTION OF SCHRODINGER EQUATION

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Abstract- The goal of this research was to examine the quantum mechanical phenomenon of tunneling with respect to the Schrödinger Equation. A quantum mechanical wave is said to "tunnel" when it travels (propagates) through a classically forbidden region. In a more physical interpretation, it is when the energy (E) of the wave is lower than the potential at a specific point V(x). [A point where V(x) is greater than E is referred to as a classical turning point.] The phenomenon of a tunneling was examined in a double-well potential. Another goal of this project was to compare two methods for approximating the tunneling time of a wave packet. The two methods used were the finite difference method and WENO approximation scheme In order to compare a potential that experienced tunneling and one that did not, the solution to a quadratic potential was also solved.

Index Terms- WENO schemes, Finite difference, Schrodinger equation, Simulation.

I. INTRODUCTION

The nonlinear Schr□dinger 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 [17] and surface waves in deep waters.
In the focusing case the NLS equation is

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

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

Such a problem belongs to the class of "integrable nonlinear equations", which means that it is solvable by the inverse scattering transform (IST) method [1,9,10]. In spite of this fact, the earlier methods but one [3] do not make use of the IST method for obtaining a numerical approximation of the exact solution of the IVP for (1). In fact, the numerical method most used is the split step Fourier method introduced by Lake et al. [12] and by Hardin and Tappert [7]. Taha and Ablowitz [14] made a comparative analysis of numerical methods to solve the IVP for (1), such as various finite-difference schemes (e.g., the Ablowitz-Ladik scheme [1], split-step Fourier methods [7] and pseudo-spectral methods [5,6] and decided in favor 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., [16]) even though in the 1990' orthogonal splines methods were successfully applied to solve the IVP for (1) [11,12,13].
In order to illustrate our contribution, let us first recall that, as found in various sources (e.g., [17, 1, 9, 2]), the solution of the IVP for (1) by the IST method is composed of the following three steps:
(1) solve the direct scattering problem for the associated Zakharov-Shabat (ZS) system to obtain the scattering data;
(2) propagate the initial scattering data in time;
(3) solve the associated inverse scattering problem, to arrive to the solution we are looking for.
Our numerical method solves the problem, allowing one to 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 numerical simulation for the resolution of the main problem.

II. SCHRODINGER EQUATION

The general one dimensional Schrödinger equation is given as follows:

$$\hat{H}\Psi(x,t)=E\Psi(x,t) \qquad (2)$$

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:

$$\hat{H}=-\nabla^2+V(x) \qquad (3)$$

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

$$-\Psi_{xx}(x,0)+V(x)\Psi(x,0)=E\Psi_t(x,0) \qquad (4)$$

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

$$-\frac{h^2}{2m}\Psi_{xx}(x,t)+V(x)\Psi(x,t)=E\Psi_t(x,t) \qquad (5)$$

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 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 mil Ψ lion 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 $\mathcal{O}$ and Ψ * or Ψ except in special cases.

III. METHODS

Finite Differences

The majority of the work was done using a finite differences approximation. Finite differences is a numerical method for solving partial an ordinary differential equations. For the Schrödinger equation, this is accomplished by spatial discretization (marching along in steps of Δx) and a matrix representation for the Hamiltonian (Equation 1.2). This approximation is:

$$K = \frac{-1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{bmatrix} + \begin{bmatrix} v_1 & & & \\ & v_2 & & \\ & & v_3 & \\ & & & v_4 \end{bmatrix}$$

Where the v_ns along the diagonal represent the potentials evaluated at the points x_n. The diagonalization of this matrix yield two matrices [V,D] where V are the eigenvectors of the K matrix stacked in columns (normal modes/stationary states -- ψ) and D is a the diagonal matrix that contain the eigenvectors ("energies" -- E) associated with the normal modes (stationary states).

WENO Method

The tunneling time for the finite differences approach was compared to the WENO (Weighted-Essentially-Non-Oscillatory) approximation method:

Finite Difference Methods are used to approximate derivate to solve differential equations numerically. The goal is to discretize the domain of the given problem, for example the x grid for a function f(x), and use the value of the function evaluated at a point and neighboring point(s) to approximate the derivative of the function at the point. The assumption made is that the functions to be differentiated are well behaved.

Then using truncated Taylor's sum, one can derive approximations for derivatives. In our project, we needed approximations for the first derivative and the second derivative.

Depending on the number of neighboring points used in approximate derivatives, we can define our approximation as being the 'three point stencil' if we are using two neighboring points along with the evaluation point, or as the five point stencil' if we are using four neighboring points along with the evaluation point and so on.

Similarly, we can define our approximations as being centered difference, backward difference, or forward difference depending upon the symmetry of the neighboring points.

Like finite differences, the WENO approximation is numerical. 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

$$S_r(i) = x_{ir},\ldots,x_{ir+k}, \qquad r = 0,\ldots,k-1 \tag{6}$$

produce k different reconstructions to the value $v_{i+1/2}$, according to (6),

$$v^{(r)}_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} c_{rj}\bar{v}_{i-r+j}, \qquad r = 0,\ldots,k-1 \tag{7}$$

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

$$v_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} w_r v^{(r)}_{i+1/2}, \tag{8}$$

We require

$$w_r \geq 0, \qquad \sum_{j=0}^{k-1} w_r = 1 \tag{9}$$

for stability and consistency.

If the function v(x) is smooth in all of the candidate stencils (6), there are constants d_r such that

$$v_{i+\frac{1}{2}} = \sum_{j=0}^{k-1} d_r v_{i+\frac{1}{2}}^{(r)} = v(x_{i+1/2}) + o(\Delta x^{2k-1}), \quad (10)$$

and for the other

$$v_{i-\frac{1}{2}} = \sum_{j=0}^{k-1} \tilde{d}_r v_{i+\frac{1}{2}}^{(r)} = v(x_{i-1/2}) + o(\Delta x^{2k-1}), \quad (11)$$

we have by symmetry

$$\tilde{d}_r = d_{k-1-r} \quad (2.11)$$

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 constancy,

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

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:

$$w_r = \frac{\alpha_r}{\sum_{s=0}^{k-1} \alpha_s}, \quad r = 0,\ldots, k-1 \quad (12)$$

with

$$\alpha_r = \frac{d_r}{(\varepsilon + \beta_r)^2} \quad (13)$$

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:

$$\beta_r = \sum_{l=0}^{k-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \Delta x^{2l-1} \left(\frac{\partial^l p_r(x)}{\partial^l x} \right) dx. \quad (14)$$

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

$$\begin{cases} \beta_0 = (\bar{v}_{i+1} - \bar{v}_i)^2, \\ \beta_1 = (\bar{v}_i - \bar{v}_{i-1})^2. \end{cases} \quad (15)$$

and for k = 3, (61) gives:

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

(16)

Now, we can form the weights w_r and $\overline{w}_r$ using (15)-(16)

and

$$\tilde{w}_r = \frac{\alpha_r}{\sum_{s=0}^{k-1} \tilde{\alpha}_s}, \qquad \tilde{\alpha}_r = \frac{\tilde{d}_r}{(\varepsilon + \beta_r)^2}. \quad (17)$$

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

$$\begin{aligned} v^+_{i+\frac{1}{2}} &= \sum_{j=0}^{k-1} w_r v_{i+\frac{1}{2}}^{(r)} \\ v^-_{i-\frac{1}{2}} &= \sum_{j=0}^{k-1} \tilde{w}_r v_{i-\frac{1}{2}}^{(r)} \end{aligned} \quad (18)$$

And now, we can return to the monotone flux chosen before for the ENO schemes then follows all the steps as in it (use (18) to compute the flux then form the WENO scheme).

RESULTS AND DISCUSSIONS

Using the finite differences methods the solutions to the Schrödinger equation were approximated by different methods. For the quadratic potential (See figure 1), the eigenvalues (energies) were equally spaced and each successive normal mode had one more node than the previous (the first normal mode, corresponding to the first eigenvalue, had the lowest energy and no nodes).

The TDSE of the quadratic potential remained inside the given potential, V(x), and did not 'tunnel' or 'go through' the potential. Instead, the wave packed turned at the classic turning points on either side of the potential (An example of a solution to the TDSE is found in figure 2).

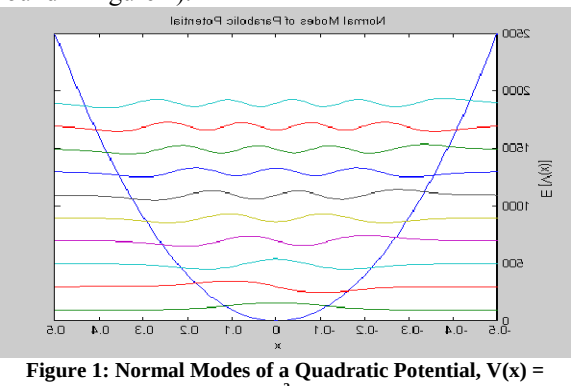


Figure 1: Normal Modes of a Quadratic Potential, V(x) = 20000x^2 [Blue]

Both real and imaginary parts of the solution are plotted.

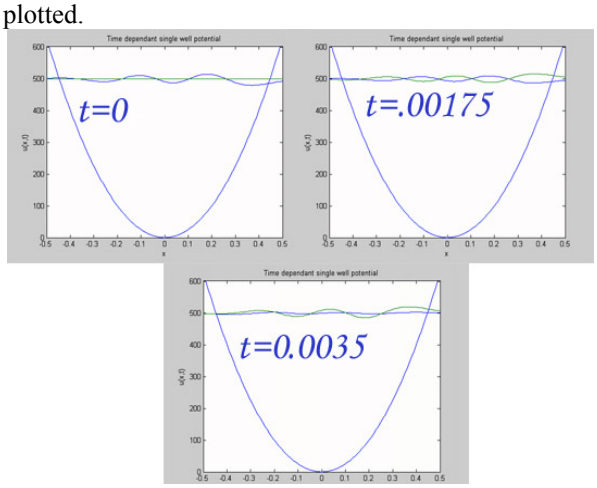


Figure 2: One solution to the TDSE. t=0 is at start of period, t=.0035 is halfway through period.

The double well (quartic) potential's normal modes had several different characteristics as compared to the double well. Firstly, the energy levels existed in pairs of closely spaced (See figure 3), nearly-degenerate doublets. These doublets in the stationary state solution arose because of the two separate wells. One of each degenerate pairs occupied one or the other well. However, they were not completely degenerate because one had to be symmetric and one had to be antisymmetric. Therefore, the symmetric level was slightly lower in energy because it had one less node than the corresponding antisymmetric level. Another interesting characteristic was the spacing of successive doublets. The spacing between successive doublets decreased as the energy was increased because of the slight anharmonicity (non-symmetric nature) of the well around the barrier. The spacing between the doublets, however, increased with increased energy until the point when E > bh when the spacing between the doublets became so large that they could be considered to be discrete normal modes.

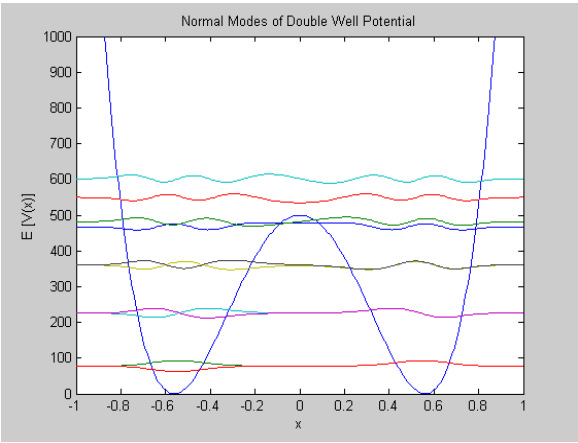


Figure 3: Normal Modes of a Double Well Potential, de V(x) = 5000x^4 - 3162x^2 + 500 [Blue]

The time evolution of a linear combination of two nearly-degenerate states was approximated using the finite differences method.

Using Weighted Essentially Non Oscillatory (WENO) on to the full time-dependent Schrödinger equation.

$$-\frac{h^2}{2m}\Psi_{xx}(x,t) + V(x)\Psi(x,t) = E\Psi_t(x,t) \qquad (19)$$

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

$$-\frac{h^2}{2m}\Psi_{xx}(x,t) = E\Psi_t(x,t) \qquad (19)$$

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

$$\Psi(x,t) = \sum_i Ae^{i(k_i x-\omega_i t)} \qquad (20)$$

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.

Starting with the initial distribution showed in the following figure 4:

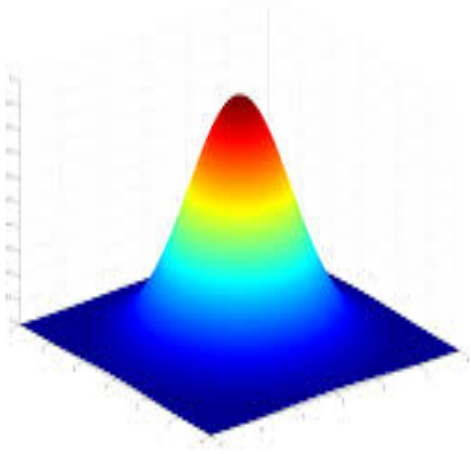


Figure 4: initial distribution function.

Along time the evolution of the distribution function at different time is shown in figure 5.

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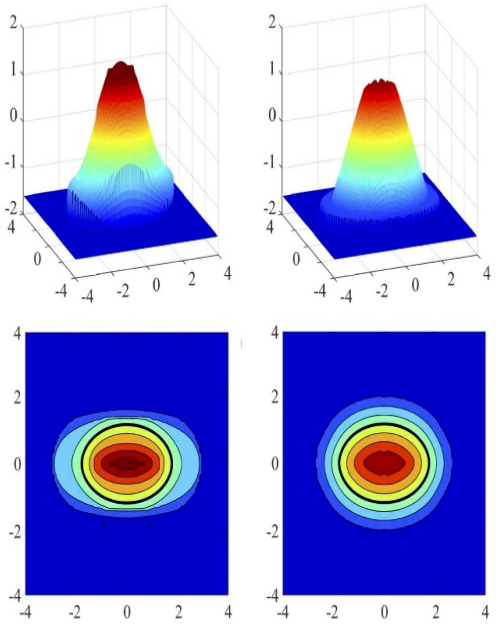


Figure 5: Time evolution of the distribution function from t=1 to t=5.

The methods agreed with each other fairly well expect for some key points. The most important disagreement is the linear combination of the lowest two doubly-degenerate pairs (x axis = 1). This is most likely due to the machine precision of the program used to calculate the energy spacing. At these low levels, the spacing between pairs is so small that the difference may only lie in the last digit or two of machine precision. This leads to less accurate energy splitting's. The other important area of divergence is the area above the barrier (x-axis = 9) because the WENO approximation only holds under the barrier when the pairs are nearly-degenerate. In the region between these points, however, when the expectation value is less than the barrier height and the machine can calculate the energy splitting's to several significant figures, the two methods correspond well and either can be used to determine the tunneling time fairly accurately.

A convergence test for the ground state energy level as well as the first energy splitting was conducted. A plot of the ground state energy level convergence is found in Figure 7, and the first energy splitting between the ground state and its nearly-degenerate pair is found in Figure 8. For both convergences, it was found that the dx values were quadratically convergent. The value of dx (Δx) actually used in previous calculations was 0.01. Though the convergence for the actually energy of the ground state is within a very narrow relative range, the convergence for the splitting occurs over a much larger range of energies. This is because, as previously stated, machine precision makes the energy splitting somewhat inaccurate at the lower levels. Perhaps, if a smaller Δx was used, the WKB and finite differences approximations would correspond better at lower energy levels.

CONCLUSION

The quantum mechanical phenomenon of tunneling can be examined using numerical and analytic methods of approximation. However, it may be useful to use both methods, depending on the conditions of the problem.

In the region when the difference between the barrier height and the energy is large (lower energy states) the best method is the WENO approximation method because of a lack of machine precision with such small energy gaps. However, when the spacing between the energy and the barrier height is very small, the better method is the well-known finite difference method because the assumptions of the WENO schemes method become no longer valid. It may also be crucial to take smaller Δx steps in order to increase the accuracy of the spacing between lower energy levels, thus increasing the accuracy of the numerical method.

REFERENCES

[1] M. J. Ablowitz and P. A. Clarkson, Solitons, nonlinear evolution equations and inverse scattering , London Mathematical Society Lecture Note Series, vol. 149, Cambridge University Press, Cambridge, 1991.

[2] M. J. Ablowitz, B. Prinari, and A. D. Trubatch, Discrete and continuous nonlinear Schr odinger systems, London Mathematical Society Lecture Note Series, vol. 302, Cambridge University Press, Cambridge, 2004.

[3] A. Arico, C. van der Mee, and S. Seatzu, Structured matrix numerical solution of the nonlinear Schr dinger equation by the inverse scattering transform , Electron. J. Differential Equations (2009), No. 15, 21.

[4] I. Daubechies, Ten lectures on wavelets , vol. 61 of CBMS-NSF Regional Conference Series in Applied Mathematics. Philadelphia, PA: Society for Industrial and Applied Mathematics (SIAM), 1992.

[5] B. Fornberg, A practical guide to pseudospectral methods , Cambridge Monographs on Applied and Computational Mathematics, vol. 1, Cambridge University Press, Cambridge, 1996.

[6] B. Fornberg and G. B. Whitham, A numerical and theoretical study of certain nonlinear wave phenomena , Philos. Trans. Roy. Soc. London Ser.A289(1978), no. 1361, 373–404.

[7] R.H. Hardin and F.D. Tappert, Applications of the split-step fourier method to the numerical solution of non-linear and variable-coefficient wave equation.

[8] S. Mallat: A wavelet Tour of Signal Processing, Academic Press, San Diego 1998

[9] S. Novikov, S. V. Manakov, L. P. Pitaevski, and V. E. Zakharov,Theory ofsolitons, Contemporary Soviet Mathematics, Consultants Bureau [Plenum], New York, 1984, The inverse scattering method, Translated from the Russian.

[10] Juuso Olkkonen; Discrete Wavelet Transforms - Theory and Applications, Intech, (2011).

[11] M. P. Robinson, The solution of nonlinear Schr dinger equations using orthogonal spline collocation, Comput. Math. Appl.33(1997), no. 7, 39–57.

[12] M. P. Robinson and G. Fairweather, Orthogonal spline collocation methods for Schr□dinger-type equations in one space variable , Numer. Math.68 (1994), no. 3, 355–375.
[13] M. P. Robinson, G. Fairweather, and B. M. Herbst, On the numerical solution of the cubic Schr□dinger equation in one space variable, J. Comput. Phys.104(1993), no. 1, 277–284.
[14] T. R. Taha and M. J. Ablowitz,Analytical and numerical aspects of certain nonlinear evolution equations. I. Analytical, J. Comput. Phys.55(1984),no. 2, 192–202.
[15] C. van der Mee, Direct and inverse scattering for skew self adjoint Hamiltonian systems, Current trends in operator theory and its applications, Oper. Theory Adv. Appl., vol. 149, Birkh □auser, Basel, 2004, pp. 407–439.
[16] J. A. C. Weideman and B. M. Herbst, Split-step methods for the solution of the nonlinear Schr□dinger equation, SIAM J. Numer. Anal.23(1986),no. 3, 485–507.
[17] V. E. Zakharov and A. B. Shabat, Exact theory of two-dimensional self-focusing and one-dimensional self-modulation of waves in non linear media, Z Eksper. Teoret. Fiz. 61(1971), no. 1, 118–134.

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