Pseudospectral Algorithms for Solving Nonlinear Schrödinger Equation in 3D

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Three pseudospectral algorithms are described (Euler, leapfrog and trapez) for solving numerically the time dependent nonlinear Schrödinger equation in one, two or three dimensions. Numerical stability regions in the parameter space are determined for the cubic nonlinearity, which can be easily extended to other nonlinearities. For the first two algorithms, maximal timesteps for stability are calculated in terms of the maximal Fourier harmonics admitted by the spectral method used to calculate space derivatives. The formulas are directly applicable if the discrete Fourier transform is used, i.e. for periodic boundary conditions. These formulas were used in the relevant numerical programs developed in our group.

I. INTRODUCTION

The nonlinear Schrödinger (NLS) equation in one, two or three dimensions is a commonly used model in various branches of physics, e.g. in plasma theory, optics or condensed matter theory. In these applications the cubic form of the nonlinear term is used, and our analysis will be pertinent to this form. However, the generalization to other nonlinearities will usually be straightforward. To make the analysis directly applicable to various situations we assume the following form of the NLS equation:

\[ i\bar{u}_t + A\bar{u}_{\bar{x}\bar{x}} + B\bar{u}_{\bar{y}\bar{y}} + C\bar{u}_{\bar{z}\bar{z}} + D|\bar{u}|^2\bar{u} + \bar{E}\bar{u} = 0, \quad (1) \]

where \(\bar{t}\) denotes time, and \(\bar{x}, \bar{y}, \bar{z}\) are space coordinates; subscripts of \(\bar{u}\) denote partial derivatives. The coefficients \(A\) (\(\neq 0\)), \(B, C, D\) (\(\neq 0\)) are assumed to be real, but \(\bar{E}\) can be complex, \(\bar{E} = \bar{E}_x + i\bar{E}_t\). The unknown function will be defined in a box:

\[ -L_\bar{x} \leq \bar{x} \leq L_\bar{x}, \quad -L_\bar{y} \leq \bar{y} \leq L_\bar{y}, \quad -L_\bar{z} \leq \bar{z} \leq L_\bar{z}, \quad (2) \]

with periodic boundary conditions: \(\bar{u}(L_\bar{x}, \ldots) = \bar{u}(-L_\bar{x}, \ldots)\), etc. These conditions will be fulfilled exactly for solutions periodic in \(\bar{x}, \bar{y}\) and \(\bar{z}\) but approximately also for solitary solutions, which are exponentially small at the boundaries. Non-periodic boundary conditions require special treatment, see the end of Sec. III.

II. TRANSFORMATION TO MACHINE UNITS

For the machine variables, which will be used in programming, we will drop the bars used in (1) to denote the original (physical) variables. Both types of variables will be linearly related to each other so as to make the NLS equation in machine units as simple as possible. As the Fourier transform of a periodic function with period \(P\) is the simplest for \(P = 2\pi\), we first transform the space intervals in (2) into the intervals \([0, 2\pi]\) by putting

\[ x = \alpha_x(\bar{x} + L_\bar{x}), \quad \alpha_x = \frac{\pi}{L_\bar{x}}, \]

\[ y = \alpha_y(\bar{y} + L_\bar{y}), \quad \alpha_y = \frac{\pi}{L_\bar{y}}, \quad (3) \]

\[ z = \alpha_z(\bar{z} + L_\bar{z}), \quad \alpha_z = \frac{\pi}{L_\bar{z}}, \]

Furthermore we normalize the time and the unknown function (\(\alpha_t, \alpha_u > 0\))

\[ t = \alpha_t \bar{t}, \quad u = \alpha_u \bar{u}. \quad (4) \]

With these transformations Eq. (1) becomes

\[ i\bar{u}_t + \frac{A\alpha_x^2}{\alpha_t}u_{xx} + \frac{B(L_\bar{x})^2}{A(L_\bar{y})^2}u_{yy} + \frac{C(L_\bar{z})^2}{A(L_\bar{z})^2}u_{zz} + \frac{\bar{E}}{\alpha_t}u = 0. \quad (5) \]

We can choose \(\alpha_t\) and \(\alpha_u\) so that \(|A|\alpha_x^2/\alpha_t = 1\) and \(|D|/(\alpha_u^2\alpha_t) = 1\), leading to

\[ \alpha_t = |A|\alpha_x^2, \quad \alpha_u = \frac{\sqrt{|D/A|}}{\alpha_x}. \quad (6) \]

With this choice Eq. (5) can be written

\[ u_t = F[u], \quad (7) \]

where

\[ F[u] = i[\text{sgn}(A)(u_{xx} + c_y u_{yy} + c_z u_{zz}) + \text{sgn}(D)|u|^2 u + \bar{E}u], \quad (8) \]
\[
c_y = \frac{B}{A} \left( \frac{L_y}{L_x} \right)^2, \\
c_z = \frac{C}{A} \left( \frac{L_z}{L_x} \right)^2, \\
E = E_r + iE_i = \frac{E}{\alpha t}.
\]  

(9)  

III. NUMERICAL ALGORITHMS

Integrating the evolution equation [14] from some value of \( t \) to a later instant \( t + \Delta t \), \( \Delta t > 0 \), we obtain

\[
u(t + \Delta t) = u(t) + \left[ F[u] \right]_t \Delta t.
\]  

(11)

Assuming that \( \Delta t \) is small, simple numerical algorithms and their error estimates can be obtained from [1] by using the parabolic interpolation formula for \( F[u] \):

\[
F[u] = F_0 + \beta(t - t) + \gamma(t - t)[\tau - (t + \Delta t)],
\]  

(12)

where the quantities \( \beta \) and \( \gamma \) can be expressed in terms of

\[
F_0 = F[u]_t, \quad F_1 = F[u]_t + \Delta t, \quad F_{1/2} = F[u]_t + \Delta t/2,
\]  

i.e.

\[
\beta = \frac{F_1 - F_0}{\Delta t}, \quad \gamma = \frac{2}{(\Delta t/2)}[F_0 - 2F_{1/2} + F_1],
\]  

(13)

\( \beta \) and \( \gamma \) are nearly independent of \( \Delta t \) (close to their limits as \( \Delta t \to 0 \)).

Inserting (12) into (11) we can find two algorithms, an Euler algorithm (first order in \( \Delta t \)):

\[
u(t + \Delta t) = u(t) + \Delta t F_0 + O[(\Delta t)^2],
\]  

(15)

a Trapez algorithm (second order in \( \Delta t \)):

\[
u(t + \Delta t) = u(t) + \Delta t \frac{1}{2} (F_0 + F_1) + O[(\Delta t)^3].
\]  

(16)

Note that (15) is an implicit algorithm: \( u(t + \Delta t) \) is defined in terms of \( u(t) \) and \( u(t + \Delta t) \), i.e. equation (16) must be solved for \( u(t + \Delta t) \). Usually, this is done by an iterative procedure, where in the lowest approximation \( F_1 \) on the RHS of (15) is replaced by \( F_0 \). This defines the first approximation to \( u(t + \Delta t) \) to be used on the RHS of (16) to define second approximation to \( u(t + \Delta t) \), etc.

Another simple (explicit) algorithm can be obtained from (16) if we put \( \tau = t + \Delta t/2 \) in (12):

\[
F_{1/2} = \frac{1}{2} (F_0 + F_1) - \gamma(\Delta t)^2/4,
\]

and use \( \frac{1}{2} (F_0 + F_1) \) calculated from this equation in (15):

\[
u(t + \Delta t) = u(t) + \Delta t F_{1/2} + O[(\Delta t)^3].
\]  

(17)

This formula defines a two-point algorithm: \( u(t + \Delta t) \) is given in terms of \( u(t) \) and \( u(t + \Delta t/2) \), i.e. at the centre of the interval \([t, t + \Delta t]\). Both \( u(t) \) and \( u(t + \Delta t/2) \) must be known, and hence the actual evolution interval is \( \Delta t/2 \) rather than \( \Delta t \). Replacing in (14) \( u(t) \to u(t - \Delta t) \), the central point will now be at \( t \), and the integration interval will be \( 2\Delta t \):

\[
u(t + \Delta t) = u(t - \Delta t) + 2\Delta t F_0 + O[(\Delta t)^3].
\]  

(18)

Here \( u(t + \Delta t) \) is defined in terms of \( u(t - \Delta t) \) and \( u(t) \). Using the known value \( u(t) \) and \( u(t + \Delta t) \) calculated from (15) we can determine \( u(t + 2\Delta t) \), etc. (the leapfrog procedure). The only problem is to start this procedure, which requires two values of \( u: u(t_0) \) and \( u(t_0 + \Delta t) \), where \( t_0 \) is an initial value of \( t \). But if \( u(t_0) \) is prescribed, the evolution equation (7) (of first order in \( t \)) defines \( u(t) \) for any \( t > t_0 \). In particular, \( u(t_0 + \Delta t) \) is defined. It can be calculated up to \( O[(\Delta t)^2] \) by using the Euler algorithm (13). Using this approximation to determine \( F[u] \) required for (15), the error in \( F[u] \) will also be \( O[(\Delta t)^2] \). After multiplication by \( \Delta t \) it will produce an error comparable with that in (15), \( O[(\Delta t)^3] \).

In the pseudospectral method described in [1], the Discrete Fourier Transform (DFT) with respect to each space variable is used to calculate the derivatives in (8). Thus the interval \([0, 2\pi] \times [0, 2\pi] \) for \( x \) will be divided into \( N_x \) subintervals of length \( \Delta x = 2\pi/N_x \), and similarly for \( y \) and \( z \). Here \( N_y \) and \( N_z \) can be either even or odd, \( N_x = 2M_x \) or \( N_x = 2M_x + 1 \), etc.). The function \( u \) defined on the discrete mesh \((x_j, y_m, z_n)\), \( j = 0, \ldots, N_x - 1 \); the numbers \( N_x, N_y \) and \( N_z \) can be either even or odd, \( N_x = 2M_x \) or \( N_x = 2M_x + 1 \), etc.). The function \( u \) defined on the discrete mesh \((x_j, y_m, z_n)\), \( j = 0, \ldots, N_x - 1 \); the numbers \( N_x, N_y \) and \( N_z \) can be either even or odd, \( N_x = 2M_x \) or \( N_x = 2M_x + 1 \), etc.)

The inverse transform is given by

\[
u(k_x) = \frac{1}{\sqrt{N_x}} \sum_{j=0}^{N_x-1} u(x_j) \exp(-ik_xx_j).
\]  

(19)

The inverse transform is given by

\[
u(k_x) = \frac{1}{\sqrt{N_x}} \sum_{k_x=-M_x}^{M_x} v(k_x) \exp(ik_x x_j) \bigg|_{x=x_j},
\]  

both if \( N_x = 2M_x \) or \( N_x = 2M_x + 1 \). In the first case, the summation index in (20) actually ends up with \( k_x = M_x - 1 \). However, as in that case \( v(k_x) \exp(ik_x x_j) \) is periodic as function of \( k_x \) with period \( 2M_x \), Eq. (20) will be correct if only one half of the contributions at \( k_x = \pm M_x \) are included in the sum over \( k_x \). Replacing \( x \to y, z \) and \( j \to m, n \) everywhere in (15) and (20) we obtain the formulas for the DFT in \( y \) (for each \( x_j \) and \( z_n \)) and in \( z \) (for each \( x_j \) and \( y_m \)). The essence of the pseudospectral approach is to calculate the partial derivatives at the mesh points by differentiating the interpolation formula (20) with respect to \( x \) (or its analogues
with respect to \( y \) or \( z \). Thus, for example
\[
    u_{xx}(x_j) = \frac{1}{\sqrt{N_x}} \sum_{k_x} (ik_x)^2 v(k_x) \exp(ik_x x_j),
\]
and similar expressions from 1999 and 2004).

As Eqs. (15), (16) and (18) (without error terms) have the same sign. Otherwise certain terms in (27) should be discarded. Nevertheless, in practice the overestimation given by the RHS of (27) in that case is not large, and if this formula is used in the expressions for maximal \( \Delta t \) for stability given in what follows, the only effect will be the introduction of a small safety margin. To obtain a precise expression for \( |w|_{\text{max}} \), all terms in (24) should be divided into two groups, of positive and negative. The contribution to the RHS of (27) of these two groups should be compared, and the group of terms with smaller contribution should be discarded.

A. Euler algorithm

Using (24) and (26) in (18) we obtain
\[
    \kappa = 1 + i\Delta t[w + iE_i],
\]
i.e.
\[
    |\kappa|^2 = 1 - 2\Delta tE_i + (\Delta t)^2[E_i^2 + w^2]
    = 1 - \Delta t[2E_i - \Delta t(E_i^2 + w^2)].
\]

Thus if \( E_i \leq 0 \), we obtain \(|\kappa|^2 > 1 \), i.e. the Euler algorithm is numerically unstable.

Numerical stability is only possible for \( E_i > 0 \) if
\[
    0 < \Delta t[2E_i - \Delta t(E_i^2 + w^2)] < 1.
\]
As in practice \(|w|_{\text{max}} \gg |E_i| \), the stability condition for the Euler algorithm takes the form
\[
    E_i > 0 \quad \text{and} \quad \Delta t < \frac{2E_i}{E_i^2 + (|w|_{\text{max}})^2},
\]
where \(|w|_{\text{max}} \) is given by (27) (with a possible modification as described above).

B. Implicit algorithm

Using (24) and (26) in (18) we obtain
\[
    \kappa = 1 - \frac{1}{2}\Delta t(E_i - iw)
    \frac{1}{1 + \frac{1}{2}\Delta t(E_i - iw)},
\]
i.e.
\[
    |\kappa|^2 = 1 - p,
    \quad p = \frac{2\Delta tE_i}{(1 + \frac{1}{2}\Delta t(E_i)^2 + (\frac{1}{2}\Delta tw)^2).}
\]

Thus if \( E_i < 0 \), we obtain \(|\kappa|^2 > 1 \), i.e. the implicit algorithm is numerically unstable, and for \( E_i = 0 \) this algorithm is marginally stable (\(|\kappa|^2 = 1 \)). And finally, for \( E_i > 0 \), \( p \) is positive and should not be greater than one (again due to expected \(|w|_{\text{max}} \gg |E_i| \)), which means numerical stability for any value of \( \Delta t \).
C. Leapfrog algorithm

Using (24) and (26) in (18) we obtain a quadratic in $\kappa$

$$\kappa^2 + 2\Delta t(E_i - iw)\kappa - 1 = 0. \quad (33)$$

Solving Eq. (33) we obtain

$$\kappa = -\Delta t(E_i - iw) \pm \sqrt{1 + (\Delta t)^2(E_i - iw)^2}. \quad (34)$$

For $E_i \neq 0$, the general expressions for the real and imaginary part of $\kappa$ are a bit complicated, but in the limit $\Delta t \to 0$ we easily find

$$\kappa \simeq \pm 1 - \Delta t(E_i + iw), \text{ i.e. } |\kappa|^2 \simeq 1 \pm 2\Delta tE_i. \quad (35)$$

This can always be greater than one, which means instability.

For $E_i = 0$, we obtain

$$\kappa = -ia \pm \sqrt{1 - a^2}, \quad a = \Delta t w. \quad (36)$$

Hence if $|a| \leq 1$ we obtain $|\kappa|^2 \equiv 1$, which means marginal stability, whereas for $|a| > 1$ we get

$$|\kappa|_{\text{max}} = |a| + \sqrt{a^2 - 1} > |a| > 1,$$

which means instability. Hence the numerical stability condition is $|a| \leq 1$. This condition leads to the following formula for maximal timestep $\Delta t$ for stability:

$$\Delta t = \frac{c}{|w|_{\text{max}}}, \quad (37)$$

where $0 < c < 1$, and $|w|_{\text{max}}$ is given by (27) (again with the possible modification).

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