Numerical approximation to solutions of linear and nonlinear Schrödinger equations

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References
The linear Schrödinger equation (LSE) plays an important role in quantum physics. It describes the evolution of the wave function of a physical system with respect to the time (Fevens and Jiang, 1999) (Griffiths, 2004). The LSE is utilized in many applications, such as light propagation in lens-like media, trapping of small particles, molecular spectroscopy and quantum electrodynamics (Gutierrez-Vega, 2007) (Guo, 2009) (Suslov, 2013a) (Suslov, 2015). Its standard form is given by

\[
i \frac{\partial \psi}{\partial t} + a \frac{\partial^2 \psi}{\partial x^2} + V \psi = 0, \tag{1}
\]

where \(a\) is a parameter depending on the modeled system and \(V\) is the coefficient related to the potential energy.
The nonlinear Schrödinger equation (NLSE) has the classical form:

\[ i \frac{\partial \psi}{\partial t} + a \frac{\partial^2 \psi}{\partial x^2} + V \psi + s |\psi|^2 \psi = 0 \]  


When \( V \neq 0 \) the equation is also known as the Gross-Pitaevskii equation (Zoller, 1997) (Carretero-Gonzalez, 2013).
Of great interest in quantum physics (Suslov, 2011a) (Suslov, 2013a) (Suslov, 2013b) (Suslov, 2015) are the nonautonomous versions of the LSE and NLSE involving the quadratic Hamiltonian operator $H$ given, in terms of $x$ and $p = -i \frac{\partial}{\partial x}$, as

$$H(x, p; t) = -a(t)p^2 + b(t)x^2 - ic(t)xp - id(t) - f(t)x - ig(t)p,$$

with $a, b, c, d, f$ and $g$ are suitable real-valued functions.
Nonautonomous LSE

The nonautonomous linear Schrödinger equation has the form

\[ i \frac{\partial \psi}{\partial t} = H(x, p) \psi. \]  \hspace{1cm} (4)

Substituting (3) in (4) yields

\[ i \psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x \]
\[ -id(t)\psi - f(t)x\psi + ig(t)\psi_x. \]  \hspace{1cm} (5)
The nonautonomous nonlinear Schrödinger equation has the form

$$i \frac{\partial \psi}{\partial t} = H(x, p)\psi + h(t)|\psi|^2\psi. \quad (6)$$

Substituting (3) in (6) yields

$$i \psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x$$
$$-id(t)\psi - f(t)x\psi + ig(t)\psi_x + h(t)|\psi|^2\psi. \quad (7)$$
Riccati/Ermakov-type system

The following system of equations and its solution was provided in (Suslov, 2008) (Suslov, 2011a) (Suslov, 2011b) with $c_0 = 0, 1$

\[
\frac{d\alpha}{dt} + b + 2c\alpha + 4a\alpha^2 = c_0 a\beta^4 \quad (8)
\]
\[
\frac{d\beta}{dt} + (c + 4a\alpha)\beta = 0 \quad (9)
\]
\[
\frac{d\gamma}{dt} + a\beta^2 = 0 \quad (10)
\]
If \( c_0 = 0 \), the system (8)-(13) is called Riccati-type system.
If \( c_0 = 1 \), the system (8)-(13) is known as Ermakov-type system.
Ansatz for the nonautonomous LSE

Lemma (Suslov (2011a))

The substitution

$$\psi(x, t) = \frac{1}{\sqrt{\mu(t)}} e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t))} u(\xi, \tau),$$

where $\xi = \beta(t)x + \epsilon(t)$ and $\tau = \gamma(t)$, transforms the nonautonomous equation

$$i\psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x$$
$$-id(t)\psi - f(t)x\psi + ig(t)\psi_x.$$  

into an autonomous form

$$-iu_\tau = -u_{\xi\xi} + c_0\xi^2 u \ (c_0 = 0, 1)$$

provided that the system (8)-(13) holds with $\alpha = \frac{1}{4a} \frac{\mu'}{\mu} - \frac{d}{2a}$. 
Ansatz for the nonautonomous NLSE

Lemma (Suslov (2015))

The nonlinear parabolic equation

\[ i\psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x \]
\[ -id(t)\psi - f(t)x\psi + ig(t)\psi_x + h(t)|\psi|^2\psi. \]

can be transformed to

\[ -iu_\tau = -u_{\xi\xi} + c_0\xi^2 u + h_0|\psi|^s\psi \quad (c_0 = 0, 1) \]

by the ansatz

\[ \psi(x, t) = \frac{1}{\sqrt{\mu(t)}} e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t))} u(\xi, \tau), \]

where \( \xi = \beta(t)x + \varepsilon(t) \) and \( \tau = \gamma(t) \), \( h = h_0 a\beta^2 \mu^s \) (\( h_0 \) constant) provided that the system (8)-(13) holds with
\[ \alpha = \frac{1}{4a}\mu' - \frac{d}{2a}. \]
Mixed norms

According to (Tao, 2006), let us define the mixed Lebesgue norms

\[ L_t^q L_x^r (\mathbb{R}^n \times I, \mathbb{C}) \]

for any interval \( I \) as the space of all functions \( u : \mathbb{R}^n \times I \rightarrow \mathbb{C} \) with norm

\[
\| u \|_{L_t^q L_x^r (\mathbb{R}^n \times I, \mathbb{C})} := \left( \int_I \| u(t) \|_{L_x^r (\mathbb{R}^n)}^q dt \right)^{1/q}
\]

\[ = \left( \int_I \left( \int_{\mathbb{R}^n} |u(x, t)|^r dx \right)^{q/r} dt \right)^{1/q}.
\]
Uniqueness of solutions

For the case $c_0 = 0$, the following result guarantees the uniqueness of the Cauchy problem involving the autonomous form of the LSE and NLSE.

Proposition (Tao (2006))

Let $I$ be a time interval containing $t_0$, and let $u, u' \in C^2_x(t \in \mathbb{R}^n \times I, \mathbb{C})$ be two classical solutions to $-iu_{\tau} = -u_{\xi\xi} + c_0\xi^2u + h_0|\psi|^s\psi$ ($c_0 = 0, 1$) with the same initial datum $u_0$ for some $h_0$ and $s$. Assume that we have the mild decay hypothesis $u, u' \in L^\infty_tL^q_x(\mathbb{R} \times I)$ for $q = 2, \infty$. Then $u = u'$. 
Description of finite difference methods

In order to avoid conditionality in the stability for the linear case, an implicit scheme (Crank-Nicolson) in time is used in order to approximate solutions for the autonomous form of the LSE. In the case of the autonomous form of the NLSE, an explicit scheme (Fourth order Runge-Kutta) is used for evolution in time in order to avoid the treatment of the nonlinear term with an implicit scheme. This makes the implementation conditionally stable and so, the number and size of time steps depend on the space discretization. A detailed analysis of the stability of this method for NLSE is carried on (Carretero-Gonzalez, 2013).
Split process

Following (Agrawal, 2007), for the Split-Step Fourier method the autonomous NLSE, with $\xi = x$ and $\tau = t$, is viewed as

$$\frac{\partial \psi}{\partial t} = (\hat{D} + \hat{N})\psi,$$

(20)

where the dispersive operator $\hat{D}$ and the nonlinear operator $\hat{N}$ are given by:

$$\hat{D} = -i \frac{\partial^2}{\partial x^2}$$

(21)

$$\hat{N} = i (c_0 \xi^2 + h_0 |\psi|^2).$$

(22)
After discretizing in time and space, the following matrix equation is obtained

\[
\left( I + \frac{ik}{2h^2} \Delta - \frac{ik}{2} [\xi]^n \right) \Psi^{n+1} = \left( I - \frac{ik}{2h^2} \Delta + \frac{ik}{2} [\xi]^n \right) \Psi^n,
\]

where \( h \) and \( k \) are the space step-size and time step-size, respectively; \( \Psi^n \) is the discrete approximation of \( \psi \) at the \( n \)-th time step, \( I \) is the identity matrix, \( \Delta \) is the discrete representation of the second derivative in space, and \([\xi]^n\) is the diagonal matrix that represents the operator of external potential, with entries \([\xi]^n_{ii} = \xi(x_i, t_n)\).
Fourth-order Runge-Kutta

According to (Carretero-Gonzalez, 2013), the Runge-Kutta scheme for NLSE is given by:

\[
\psi_{n+1} = \psi_n + \frac{1}{6}k(m_1 + 2m_2 + 2m_3 + m_4)
\]

\[
m_1 = F(\psi^n)
\]

\[
m_2 = F(\psi^n + \frac{1}{2}km_1)
\]

\[
m_3 = F(\psi^n + \frac{1}{2}km_2)
\]

\[
m_4 = F(\psi^n + km_3)
\]

where \(F(\psi^n) = \left(\frac{-i}{\hbar^2} \Delta + \frac{i}{\hbar^2} [\xi] + \frac{i\hbar_0}{\hbar^2} [||\psi^n||^2]\right) \psi^n\).

\(I\) is the identity matrix and \([||\psi^n||^2]\) is a diagonal matrix where \(\left[||\psi^n||^2\right]_{i,i} = \left|\psi_{x_i}^n\right|^2\).
Split-step Fourier method

The method assumes that, over a small time-step, the operators \( \hat{D} \) and \( \hat{N} \) act independently (Agrawal, 2007),

\[
\psi^{n+1} = \exp \left( \frac{k}{2} \hat{D} \right) \exp(\tau \hat{N}) \exp \left( \frac{k}{2} \hat{D} \right) \psi^n. \tag{23}
\]

The linear step has a solution in the Fourier domain. So, Fourier transform is used:

\[
\exp(k \hat{D})\psi = F_T^{-1} \exp[ik \hat{D}(\omega^2)]F_T \psi,
\]

where \( F_T \) is the Fourier transform. The term \( i \hat{D}(\omega^2) \) is obtained from \( \frac{\partial^2}{\partial x^2} \) by replacing \( \frac{\partial}{\partial x} \) by \( -i\omega \). \( \omega \) is the frequency in the Fourier domain (wave number).

Discrete Fast Fourier Transform is used to compute the Fourier transform and inverse Fourier transform.
Some exact solutions to the following paraxial wave equation are given in (Suslov, 2013b)

\[ 2i\psi_t = \psi_{xx} + x^2\psi. \]  

(24)

Exact solutions are expressed by

\[ \psi_n(x, t) = e^{i(\alpha x^2 + \delta x + \kappa) + i(2n+1)\gamma} \sqrt{\frac{\beta}{2^n n! \sqrt{\pi}}} e^{-(\beta x + \varepsilon)^2/2} H_n(\beta x + \varepsilon), \]

where

\[ \alpha(t) = \frac{\alpha(0)\cos 2t + \sin 2t(\beta^4(0) + 4\alpha^2(0) - 1)/4}{\beta^4(0)\sin t + (2\alpha(0)\sin t + \cos t)^2}, \]
\[ \beta(t) = \frac{\alpha(0)\cos 2t + \sin 2t(\beta^4(0) + 4\alpha^2(0) - 1)/4}{\beta^4(0)\sin t + (2\alpha(0)\sin t + \cos t)^2}, \]
\[ \gamma(t) = -\frac{1}{2} \arctan \frac{\beta^2(0)\tan t}{1 + 2\alpha(0)\tan t}, \]
\[ \delta(t) = \frac{\delta(0)(2\alpha(0)\sin t + \cos t) + \varepsilon(0)\beta^3(0)\sin t}{\beta^4(0)\sin^2 t + (2\alpha(0)\sin t + \cos t)^2}, \]
\[ \varepsilon(t) = \frac{\varepsilon(0)(2\alpha(0)\sin t + \cos t) - \beta(0)\delta(0)\sin t}{\sqrt{\beta^4(0)\sin^2 t + (2\alpha(0)\sin t + \cos t)^2}}, \]
\[ \kappa(t) = \sin^2 t \frac{\varepsilon(0)\beta^2(0)(\alpha(0)\varepsilon(0) - \beta(0)\delta(0)) - \alpha(0)\delta^2(0)}{\beta^4(0)\sin^2 t + (2\alpha(0)\sin t + \cos t)^2}, \]

with \( \alpha(0) = \gamma(0) = \varepsilon(0) = \kappa(0) = 0, \ n = 0, \ \delta(0) = 0, 1, \ \beta(0) = 4/9. \)
Numerical solution to the equation $2i\psi_t = \psi_{xx} + x^2\psi$ with the parameter $\delta(0) = 0$. 
Numerical solution. Case $\delta(0) = 1$

Numerical solution to the equation $2i\psi_t = \psi_{xx} + x^2\psi$ with the parameter $\delta(0) = 1$. 
The following equation was considered for the NLSE

\[ i\psi_t = -a\psi_{xx} - |\psi|^2\psi. \]  \hspace{1cm} (25)

The exact solution is given in (Rajendran, 2010) with

\[ \psi(x, t) = A \text{sech} \left[ \frac{A}{\sqrt{2}} (x - \Omega t) \right] \exp \left[ i \left( \frac{\Omega}{2} x + \frac{2A^2 - \Omega^2}{4} t \right) \right], \]

corresponding to a bright soliton solution.

If \( A = \sqrt{2} \) and \( \Omega = 0 \), then it yields

\[ \psi(x, t) = \sqrt{2} \text{sech}[x] e^{it}. \]
Numerical solution to the equation $i\psi_t = -a\psi_{xx} - |\psi|^2\psi$ with the parameters $A = \sqrt{2}$ and $\Omega = 0$. 
Numerical solution to the equation $i\psi_t = -a\psi_{xx} - |\psi|^2\psi$ with the parameters $A = -1.8$ and $\Omega = 4$. 
For the equation

\[ i\psi_t = -a\psi_{xx} + |\psi|^2\psi, \]  

(26)

with solution given in (Escorcia, 2014) by

\[ \psi(x, t) = \frac{1}{\sqrt{2}} [v - 2iA \tanh A(x - \Omega t)] \exp \left[ -\frac{i}{2} (v^2 + 4A^2) t \right], \]

corresponding to a dark soliton-type solution. If \( A = 1/2 \) and \( \Omega = 0 \), this yields

\[ -\frac{1}{\sqrt{2}} \tanh \left( \frac{1}{2} x \right) \exp \left( -\frac{i}{2} t \right). \]
Numerical solution. Case $A = 1/2$, $\Omega = 0$.

Numerical solution to the equation $i\psi_t = -a\psi_{xx} + |\psi|^2\psi$ with the parameters $A = 1/2$ and $\Omega = 0$. 
Ongoing work

- To explore more methods to get an optimal approximation to the nonautonomous NLSE.
- To validate the results obtained when considering more general forms of the coefficients in the nonautonomous form of the LSE and NLSE (nonexplicit solutions and generalized functions).
- To extend the previous results for the LSE and the NLSE on two-dimensional domains, and compare them with exact solutions like...


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Thank you!