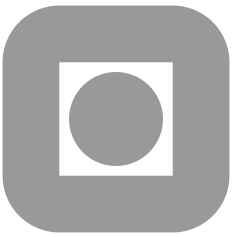
NORGES TEKNISK-NATURVITENSKAPELIGE
UNIVERSITET

Symmetric exponential integrators for the cubic Schrödinger equation

by

Elena Celledoni, David Cohen, Brynjulf Owren

PREPRINT
NUMERICS NO. 3/2006



NORWEGIAN UNIVERSITY OF
SCIENCE AND TECHNOLOGY
TRONDHEIM, NORWAY

This report has URL
http://www.math.ntnu.no/preprint/numerics/2006/N3-2006.pdf
Address: Department of Mathematical Sciences, Norwegian University of Science and Technology, N-7491 Trondheim, Norway.

Symmetric exponential integrators for the cubic Schrödinger equation

Elena Celledoni, David Cohen, Brynjulf Owren

November 27, 2006

1 Introduction

The cubic Schrödinger equation in $\mathbf{T}^d$ is

$$\mathrm{i}u_t + \Delta u = \lambda |u|^2 u. \tag{1}$$

For $d = 1$, this equation is completely integrable and in general it has the L^2-norm or density as a conserved quantity

$$\rho[u] = \int_{\mathbf{T}^d} |u|^2 \, \mathrm{d}\mathbf{x} \tag{2}$$

and for H^1-solutions one has conservation of energy

$$H[u] = \int_{\mathbf{T}^d} \left(\frac{1}{2} |\nabla u|^2 + \frac{\lambda}{4} |u|^4 \right) \mathrm{d}\mathbf{x}. \tag{3}$$

It is of great interest [6, 8] to devise numerical schemes which conserve discretized versions of these same invariants. In practice one needs to introduce a space discretization of (1) and in the periodic case, the use of a discrete Fourier transformation is a favourable choice. Several methods have been proposed for the numerical integration of the cubic Schrödinger equation. For arbitrary d, examples of schemes which exactly preserve (2), (3) or discretized versions of them, are those by [9], [4]. Special attention has been given to the one-dimensional case. Considerable success has been reported in early papers using splitting and Fourier techniques, see [19] for a review and comparisons. Another approach has been to impose integrability on the discrete level, the best example is the Ablowitz-Ladik model [1], its numerical properties are discussed in [12]. The Hamiltonian structure of nonlinear wave equations in general and the cubic Schrödinger equation in particular has invoked the idea of applying symplectic time integrators to semidiscretizations of these equations, see e.g. McLachlan [16]. More recently, the use of multisymplectic formulations of Hamiltonian wave equations has become popular as a basis for designing numerical schemes with good geometric properties. For the cubic Schrödinger equation, schemes that preserve a discretized version of the multisymplectic form were discussed by Reich [18]. In multisymplectic integration, there are also local conservation of quantities derived from the multisymplectic form, like energy and momentum. When discretizing in space, and imposing conservation of a space averaged quantity, one may observe large local fluctuations in space that are averaged throughout the domain. In [13] Islas and Schober consider properties of the nonlinear spectrum for a certain initial function in the cubic Schrödinger equation, in particular they study whether a small gap in this invariant spectrum is closed

by the numerical scheme. The multisymplectic schemes seem to handle this problem well, however in a more recent report [2] it was pointed out that these spectral properties were also very well conserved by another type of time integration scheme called exponential integrators. Modern versions of these schemes are generally formulated for problems of the form

$$\dot{u} = L\,u + N(u). \tag{4}$$

Here L is typically a linear unbounded differential operator, alternatively one can think of L as a matrix arising from a space discretization of such an operator and thus bounded for a fixed spatial resolution, but with a large norm. The map $N(u)$ is on the other hand nonlinear, but we assume that for spatial resolutions of interest the size of N is small compared to L. The schemes we consider here can all be cast in the form

$$N_r = N(\mathrm{e}^{c_r hL}\,u_0 + h\sum_j a_{rj}(hL)N_j), \quad r = 1,\ldots,s \tag{5}$$

$$u_1 = \mathrm{e}^{hL}\,u_0 + h\sum_r b_r(hL)N_r \tag{6}$$

Here the functions $a_{rj}(z)$ and $b_r(z)$ are usually real entire or at least real analytic in a domain of the complex plane which includes the spectrum of hL for all h of interest. Their value at 0, $a_{rj} := a_{rj}(0)$ and $b_r := b_r(0)$ is the underlying Runge-Kutta method to which the scheme reduces in situation that $L = 0$ in (4). One then has $c_r = \sum_j a_{rj}$. In applying such schemes to the nonlinear Schrödinger equation, it is of importance to choose functions $a_{rj}(z)$ and $b_r(z)$ which are bounded on the imaginary axis, a property which is rather common among popular exponential integrators. Although we shall not dwell too much on the added technical difficulties related to the situation when the problem (4) is infinite dimensional, it deserves a few remarks. In the present situation we are interested in the case where $L = \mathrm{i}A$ with A a self-adjoint operator on the Hilbert space $L^2(\mathbf{T}^d)$. In this case L is the infinitesimal generator of a one-parameter unitary group. The spectrum of L is on the imaginary axis and we assume that functions $f(hL)$ can be defined in terms of eigenvalues λ_i of L and a complete set of orthonormal eigenvectors e_i through the spectral mapping theorem as

$$f(hL)u = \sum_i f(\lambda_i)\langle u, e_i\rangle\, e_i$$

where f satisfies the requirements stated above for $a_{rj}(z)$ and $b_j(z)$.

Exponential integrators go back a long time, at least to Certaine [7], but there has been a revived interest in these schemes in the last decade, for an account see for instance [17] and the references therein. Most of the recently proposed exponential integrators have the property that $a_{rj}(z) \equiv 0$ for $j \geq r$ and are thus explicit in the nonlinear term $N(u)$. For periodic problems, the Fourier transformation diagonalizes the operator L making the functions $a_{rj}(hL)$ and $b_r(hL)$ inexpensive to compute and store. For constant stepsize they can even be reused in every step. A disadvantage with such schemes is that they cannot be symplectic or symmetric. However, in the related class of schemes called Lie group integrators, implicit schemes that are self adjoint were considered by Zanna et al. [20]. In this work we shall consider implicit schemes of the form (5), (6) that are symmetric. We shall argue that the implicitness is still relatively inexpensive to handle and that we obtain methods with good long time preservation properties. We show however that the schemes cannot in general preserve quadratic invariants exactly, and in particular the density $\rho[u]$. But it is possible to force exact preservation without the loss of symmetry by using the symmetric projection approach as discussed by Hairer [10]. We show how this projection

can be implemented at relatively low additional cost. Finally, we illustrate the behaviour of these new schemes by numerical experiments.

2 Symmetric exponential integrators

Writing $u_1 = \Phi_h(u_0)$ for the exponential integrator defined in the introduction, one defines the adjoint method as the map

$$^*\Phi_h = \Phi_{-h}^{-1}.$$

A straightforward calculation (exchanging $1 \leftrightarrow 0$ and $h \leftrightarrow -h$, as usual) shows that the adjoint scheme $^*\Phi_h$ is again a scheme of the form (5)-(6) where the coefficient functions $^*a_{rj}(z)$ and $^*b_r(z)$ are given as

$$^*a_{rj}(z) = \mathrm{e}^{(1-c_{s+1-r})z}\, b_{s+1-j}(-z) - a_{s+1-r,s+1-j}(-z) \tag{7}$$

$$^*b_r(z) = \mathrm{e}^{z}\, b_{s+1-r}(-z). \tag{8}$$

We now consider the possibility of obtaining symmetric methods, i.e. schemes where $^*a_{rj}(z) = a_{rj}(z)$, $^*b_r(z) = b_r(z)$.

Symmetric one-stage exponential integrators If $s = 1$ there is only $a(z) := a_{11}(z)$, $b(z) := b_1(z)$, $c := c_1 = a_{11}(0)$ to be determined. We get immediately from (7)-(8) that

$$a(z) = \mathrm{e}^{(1-c)z}\, b(-z) - a(-z) \tag{9}$$

$$b(z) = \mathrm{e}^{z}\, b(-z). \tag{10}$$

So by multiplying (10) from each side by $\mathrm{e}^{-z/2}$ we realize that $G(z) := \mathrm{e}^{-z/2} b(z)$ must be an even function so that

$$b(z) = \mathrm{e}^{z/2}\, G(z), \quad G(z) \text{ even}, \ G(0) = 1.$$

Combining (9) and (10) we derive

$$a(z) + a(-z) = \mathrm{e}^{-cz} b(z) = \mathrm{e}^{(\frac{1}{2}-c)z} G(z),$$

thus $c = \frac{1}{2}$, and the even part of $a(z)$ equals $G(z)/2$. Summarizing, a one stage symmetric exponential integrator is constructed as follows

- Let $c = \frac{1}{2}$ and choose $a(z)$ arbitrary, subject only to the condition $a(0) = \frac{1}{2}$.
- Set $b(z) = \mathrm{e}^{z/2}(a(z) + a(-z))$.

Note in particular that every one stage symmetric exponential integrator will have the midpoint rule as its underlying scheme.

An example can be written as follows

$$U = \mathrm{e}^{\frac{hL}{2}}\, u_0 + \frac{h}{2}\, \varphi_1(\frac{hL}{2})\, N(U) \tag{11}$$

$$u_1 = \mathrm{e}^{hL}\, u_0 + h\, \varphi_1(hL)\, N(U). \tag{12}$$

Alternatively, the update step can be written as

$$u_1 = \mathrm{e}^{\frac{hL}{2}}\, U + \frac{h}{2}\, \varphi_1(\frac{hL}{2})\, N(U), \tag{13}$$

with $\varphi_1(z) = \frac{\mathrm{e}^z - 1}{z}$ (see [17], for details on the φ_l functions).

Symmetric two-stages exponential integrators To illustrate the case with two stages, we use the Hammer and Hollingsworth method (a Gauss method with $s = 2$) as an underlying scheme:

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

Of the six conditions (7)-(8) only three are independent. Subject to the obvious condition on the coefficient functions at $z = 0$ we can use the following recipe to obtain a two-stage symmetric exponential integrator

- Pick $b_1(z)$ arbitrarily and set $b_2(z) = \mathrm{e}^z\, b_1(-z)$.
- Pick $a_{11}(z)$ arbitrarily and set $a_{22}(z) = e^{c_2 z} b_1(-z) - a_{11}(-z)$.
- Pick $a_{12}(z)$ arbitrarily and set $a_{21}(z) = e^{-c_1 z} b_1(z) - a_{12}(-z)$.

We have not pursued any further the question of how to best make use of this freedom to find optimal symmetric schemes with two stages. It however not difficult to see that the two-stages Lawson method (see [14]) having coefficients

$$a_{rj}(z) = \alpha_{rj}\mathrm{e}^{(c_r - c_j)z}, \quad b_r(z) = \beta_r \mathrm{e}^{(1-c_r)z}$$

actually satisfy (7) and (8) if the underlying Runge-Kutta with coefficients α_{rj} and β_r is the method of Hammer and Hollingsworth.

Symmetric Lawson methods We will now give a complete characterization of the symmetric Lawson methods. The Lawson methods are symmetric if

$$\begin{aligned} a_{rj}(z) &= \mathrm{e}^{(1-c_{s+1-r})z}\, b_{s+1-j}(-z) - a_{s+1-r,s+1-j}(-z) \\ b_r(z) &= \mathrm{e}^z\, b_{s+1-r}(-z). \end{aligned}$$

Recalling the definition of the coefficient functions $a_{rj}(z)$ and $b_r(z)$ of a Lawson scheme, we obtain symmetry if

$$\begin{aligned} \alpha_{r,j}\, \mathrm{e}^{(c_r - c_j)z} &= (\beta_{s+1-j} - \alpha_{s+1-r,s+1-j})\, \mathrm{e}^{(c_{s+1-j} - c_{s+1-r})z} \\ \beta_r\, \mathrm{e}^{(1-c_r)z} &= \beta_{s+1-r}\, \mathrm{e}^{c_{s+1-r} z}. \end{aligned}$$

We thus obtain the following result (which can be compared to the result on symmetric Runge-Kutta, see [11, Sect. V.2])

Proposition 2.1. *The Lawson method with coefficients*

$$a_{rj}(z) = \alpha_{rj}\mathrm{e}^{(c_r - c_j)z}, \quad b_r(z) = \beta_r \mathrm{e}^{(1-c_r)z}$$

is symmetric if the underlying Runge-Kutta method with coefficients α_{rj}, β_r verify

$$c_{s+1-r} = 1 - c_r, \quad \beta_{s+1-r} = \beta_r, \quad \beta_j = \alpha_{r,j} + \alpha_{s+1-r,s+1-j} \quad \textit{for all} \quad r, j.$$

3 L^2-norm preservation for the nonlinear Schrödinger equation

We know (see for example [15]) that the L^2-norm $||u(\cdot,t)||_{L^2}$ of the exact solution of the nonlinear Schrödinger equation is a conserved quantity.

The aim of geometric numerical integration is to retain by a numerical discretization as much as possible of the geometric structure of the exact solution. It is thus natural to require that the L^2-norm of the numerical solution, given by the exponential integrators (5)–(6), to be preserved.

We will now give a complete characterization of the exponential integrators which conserve exactly quadratic invariants of the form $\rho[u] = \langle u, u\rangle$.

Proposition 3.1. *Consider the class of problems $\dot{u} = Lu + N(u)$ where $\mathrm{i}L$ is self-adjoint and where $\rho[u] = \langle u, u\rangle$ is preserved. An exponential integrator with coefficient functions $a_{rj}(z)$ and $b_r(z)$ of the exponential integrator will preserve $\rho[u]$ for* all *problems in this class if there are real numbers $\beta_1, \ldots, \beta_s$ such that*

$$b_r(hL) = \beta_r \, \mathrm{e}^{(1-c_r)hL}, \;\; r = 1, \ldots, s \tag{14}$$

$$\beta_j \beta_r \, \mathrm{e}^{(c_j - c_r)hL} = \beta_j \, a_{jr}(hL) + \beta_r \, a^*_{rj}(hL), \;\; r, j = 1, \ldots, s. \tag{15}$$

Here $a^*(hL)$ is the adjoint of $a(hL)$.

Proof. We first calculate from (6) writing just b_r for $b_r(hL)$ and using that e^{hL} is unitary

$$\langle u_1, u_1\rangle = \langle u_0, u_0\rangle + h \sum_r (\langle \mathrm{e}^{hL} u_0, b_r N_r\rangle + \langle b_r N_r, \mathrm{e}^{hL} u_0\rangle) + h^2 \sum_{r,j} \langle b_r N_r, b_j N_j\rangle$$

writing $N_r = N(U_r)$ in (5) we substitute

$$\mathrm{e}^{hL} u_0 = \mathrm{e}^{(1-c_r)hL} \, U_r - h \sum_j \mathrm{e}^{(1-c_r)hL} \, a_{rj} N_j$$

to obtain

$$\begin{aligned} \rho[u_1] - \rho[u_0] = {} & 2\,h \sum_r \mathrm{Re}\, \langle b^*_r \, \mathrm{e}^{(1-c_r)hL} \, U_r, N_r\rangle \\ & + h^2 \sum_{r,j} \langle (b^*_j b_r - b^*_j \mathrm{e}^{(1-c_j)hL} a_{jr} - a^*_{rj} \mathrm{e}^{-(1-c_r)hL} b_r) \, N_r, N_j\rangle. \end{aligned} \tag{16}$$

Note that for the exact solutions it holds for any u that

$$\frac{d}{dt}\rho[u] = 2\mathrm{Re}\, \langle u, N(u)\rangle = 0.$$

It easily follows from (16) that (14) and (15) imply $\rho[u_1] = \rho[u_0]$. □

Remarks:

1. *To consider the converse of this result, one needs to look at the notion of irreducibility for exponential integrators. If it can be asserted that each term must vanish in the two sums of* (16) *then the conditions* (14), (15) *are also necessary.*

2. *For the symmetric midpoint exponential integrator, the double sum of* (16) *vanishes, however the other one does not. Thus the numerical solution given by this method will not preserve exactly the $\rho[u]$ as we will see in Section 6*

3. *The proof of Proposition 3.1 does not apply to the conservation of quadratic invariants of the more general form $\langle u, Cu\rangle$. Indeed, to obtain the term $\langle u_0, u_0\rangle$, we have to assume that $(C\mathrm{e}^{hL})^* = C\mathrm{e}^{-hL}$, which is, in general, not possible.*

We note that the methods proposed by Lawson (see Section 2) actually satisfy (14), (15) whenever α_{rj}, β_r, of the underlying Runge-Kutta scheme are chosen to satisfy the conditions

$$\beta_r\beta_j = \beta_j\,\alpha_{jr} + \beta_r\,\alpha_{rj}, \qquad \text{for} \qquad r, j = 1, \ldots, s.$$

In fact, the Lawson schemes can be interpreted as applying a classical Runge-Kutta scheme to the differential equation resulting from the change of variables

$$y(t) = \mathrm{e}^{(t-t_0)L}v(t) \qquad \Rightarrow \qquad v'(t) = \mathrm{e}^{-(t-t_0)L}N(\mathrm{e}^{(t-t_0)L}v(t)).$$

This observation suggests that one may in fact replace the transformation used in the Lawson scheme by any unitary transformation and consider the integrator resulting from applying a classical quadratic invariant preserving scheme to the transformed system. An example of a transformation which could be used is the Cayley transform.

4 Symmetric projection algorithm

Following Hairer [10], one may perform a symmetric projection of the symmetric exponential integrator onto the constraint manifold. Suppose a constraint map $P : \mathbf{R}^m \to \mathbf{R}^q$ is given such that there are q preserved quantities $P_k(u) = 0,\ k = 1, \ldots, q$. The idea is to perturb the initial value u_0 away from the constraint manifold, apply a step of a symmetric scheme and then project back in such a way that the three composed steps give a symmetric map. Denoting by Φ_h the symmetric integrator, we have

$$\begin{aligned}
\tilde{u}_0 &= u_0 + P'(u_0)^T\,\mu \\
\tilde{u}_1 &= \Phi_h(\tilde{u}_0) \\
u_1 &= \tilde{u}_1 + P'(u_1)^T\,\mu
\end{aligned}$$

where $\mu \in \mathbf{R}^q$ is chosen such that $P(u_1) = 0$. Here $P'(u) \in \mathbf{R}^{q\times m}$ is the Jacobian matrix evaluated at the point $u \in \mathbf{R}^m$. Considering the midpoint rule (11), (13) we write the symmetric projection method on the form

$$\begin{aligned}
U - \mathrm{e}^{\frac{hL}{2}}(u_0 + P'(u_0)^T\mu) - \frac{h}{2}\,\phi_1(\frac{hL}{2})\,N(U) &= 0 \\
u_1 - \mathrm{e}^{\frac{hL}{2}}U - \frac{h}{2}\,\phi_1(\frac{hL}{2})\,N(U) - P'(u_1)^T\mu &= 0 \\
P(u_1) &= 0
\end{aligned}$$

This is now a coupled system of $2m + q$ equations $F(Y) = 0$ for the unknowns $Y = (U, u_1, \mu)$. Thus it seems that the situation with respect to computational complexity has deteriorated considerably. However, we may approximate the Jacobian matrix of F by the matrix

$$J = \begin{bmatrix} I_m & 0 & -\mathrm{e}^{hL/2}\,P'(u_0)^T \\ -\mathrm{e}^{hL/2} & I_m - P''(u_1, \mu) & -P'(u_1)^T \\ 0 & P'(u_1) & 0 \end{bmatrix}$$

Here I_m is the $m \times m$ identity matrix and $P''(u, \mu)$ is the Jacobian matrix of $P'(u)^T\mu$ with respect to u. If one only projects onto the density constraint, this matrix is simply a

scalar times I_m. In the case of projection onto both the density and the energy constraint one may replace this second derivative matrix with a simple linearization, disregarding the contributions due to the nonlinear map N. As a result the submatrix corresponding to the four left uppermost blocks of J, becomes easy to invert. Thus the kth iterate for the increment of the Lagrange multiplier μ can be calculated efficiently by means of a Schur complement formula, followed by a sequential calculation of the iterate for U and u_1.

5 Implementation issues

One needs to solve the equation

$$U = g(U) := \mathrm{e}^{\frac{hL}{2}}\, u_0 + \frac{h}{2}\, \varphi_1(\frac{hL}{2})\, N(U) \tag{17}$$

with respect to U. One may apply fixed point iteration directly to (17), to obtain approximations $U^{[k]}$ to U

$$U^{[k+1]} = \mathrm{e}^{\frac{hL}{2}}\, U_0 + \frac{h}{2}\, \varphi_1(\frac{hL}{2})\, N(U^{[k]}).$$

By defining the iteration error $e^{[k]} = U^{[k]} - U$ one gets the recursion

$$e^{[k+1]} = \frac{h}{2}\, \varphi_1(\frac{hL}{2}) \left(N(U^{[k]}) - N(U) \right) \approx \frac{h}{2}\, \varphi_1(\frac{hL}{2})\, N'(U)\, e^{[k]}.$$

The derivative map $N'(U)$ can be bounded in a strip containing the solution and the bound is obtained independently of the dimension of the discretized system. Using the discrete Fourier transformation, $\varphi_1(\frac{hL}{2})$ is a diagonal matrix whose norm is bounded by 1.

In order to further improve the convergence properties, one may consider the exact Newton iteration for solving (17)

$$U^{[k+1]} = U^{[k]} - \left[I - g'(U^{[k]}) \right]^{-1} r^{[k]}, \qquad r^{[k]} = U^{[k]} - g(U^{[k]}).$$

Noting that $g(U) = \mathcal{O}(h)$ we can approximate

$$\left[I - g'(U^{[k]}) \right]^{-1} \approx I + g'(U^{[k]})$$

and thus obtain the iteration

$$U^{[k+1]} = g(U^{[k]}) - g'(U^{[k]})\, r^{[k]}.$$

In the cubic Schrödinger equation one has $N(u) = -\mathrm{i}\lambda |u|^2\, u$ which leads to

$$N'(u)\, v = -\mathrm{i}\lambda \left(2\, |u|^2\, v + u^2\, \overline{v} \right).$$

Using a pseudospectral discretization, we replace $N(u)$ by the function

$$\hat{N}(\hat{u}) = \mathcal{F}(N(\mathcal{F}^{-1}(\hat{u})))$$

and the derivative map is

$$\hat{N}'(\hat{u})\hat{v} = \mathcal{F} \left(N'(\mathcal{F}^{-1}\hat{u})\, \mathcal{F}^{-1}\hat{v} \right).$$

Note however that when $\hat{N}'(\hat{U}^{[k]})\, \hat{r}^{[k]}$ is required, one has already computed $U^{[k]} = \mathcal{F}^{-1}\hat{U}^{[k]}$ as a part of the residual calculation, and thus only two additional Fourier transforms are required for this modification. More advanced algorithms for approximating the Newton iteration map could of course be devised, for instance by Krylov subspace techniques.

6 Numerical experiments

We illustrate the results of the preceding sections with some numerical experiments. In this section, we will present some results on the cubic Schrödinger equation (1) setting $d = 1$ and $\lambda = -1$, with periodic boundary conditions, integrated from 0 to T. We consider a pseudospectral space discretization and two different choices for the initial condition. The first is

$$u(x, 0) = 1/(1 + \sin(x)^2), \tag{18}$$

whereas the second is

$$u(x, 0) = \sqrt{8}/\cosh(2x)\mathrm{e}^{2\mathrm{i}x}, \tag{19}$$

a soliton solution. The initial data (19) require smaller time steps than (18). In these experiments we always choose a pseudospectral discretization in space with $M = 512$ Fourier modes. The stepsizes h we use always satisfy $hM^2 \gg 1$ meaning that we operate far away from the regime of explicit integrators.

In the following we plot the error of the numerical methods in the preservation of the discretized invariants corresponding to (2) and (3),

$$\rho_{\Delta x}[U] = \frac{2\pi}{M} \sum_{k=1}^{M} |U_k|^2,$$

and

$$H_{\Delta x}[U] = \frac{\pi\lambda}{2M} \sum_{k=1}^{M} |U_k|^4 + \frac{M}{4\pi} \sum_{k=1}^{M} |U_{k+1} - U_k|^2,$$

respectively. The considered numerical schemes are:

1. The symmetric midpoint exponential integrator (11)–(12) of the second section (SM-EXP). This method is symmetric but does not preserve quadratic invariants.

2. The one-stage Lawson scheme (L1) with coefficients

   $$a_{11}(z) = 1/2,\ b_1(z) = \mathrm{e}^{z/2}, \quad \text{and} \quad c_1 = 1/2.$$

   A symmetric and quadratic invariant preserving method.

3. The symmetrically projected midpoint exponential integrator, with projection on the density constraint (SPMEXP-D), and with projection on both the density and energy constraint (SPMEXP-DE). The constraint map P of section 4 in this case is $P(U) = \rho_{\Delta x}[U] - \rho_{\Delta x}[U_0]$ for (SPMEXP-D), and

   $$P(U) = \begin{bmatrix} \rho_{\Delta x}[U] - \rho_{\Delta x}[U_0] \\ H_{\Delta x}[U] - H_{\Delta x}[U_0] \end{bmatrix},$$

   for (SPMEXP-DE). The method (SPMEXP-D) preserves exactly the discrete density, and the method (SPMEXP-DE) preserves exactly both the discrete density and the discrete energy.

4. The Pseudo-Steady-State-Approximation (PASSA) scheme (see [3] and references therein). This exponential type method is a standard scheme in the chemistry literature, has order two and is not symmetric.

5. A relaxation scheme proposed by Besse in [4] (B).

6. The multisymplectic concatenated midpoint rule also known as the Preissman box scheme (MULTI). See Islas, Karpeev and Schober [12] for a thorough discussion of this method applied to the cubic Schrödinger equation (see also [5]).

Figure 1 shows the error in the discretized energy and density along the numerical solution given by (SMEXP), (L1) and (PASSA) obtained with a constant step size $h = 0.1$ for the first choice of initial value, the interval of integration is $[0, 500]$.

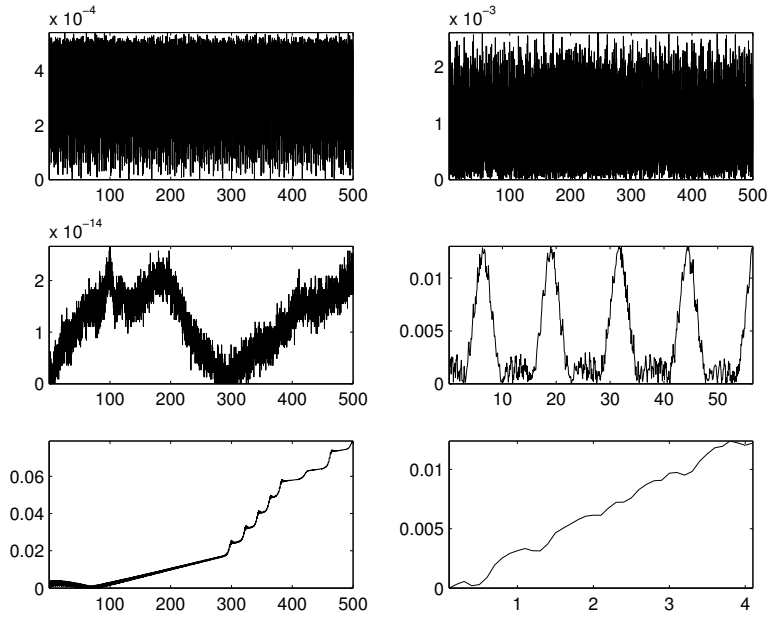


Figure 1: Density (left column) and energy along (SMEXP), (L1) and (PASSA) (from the top to the bottom) for the initial condition (18). Number of Fourier modes $M = 512$, time step 0.1.

As predicted by Proposition 3.1, the Lawson scheme preserves exactly the discretized density, which is not the case for the symmetric exponential integrator. This last scheme seems, however, to have good conservation properties.

For the soliton solution we have to use a smaller step size. Figure 2 shows as before energy and density error for the second choice of initial value and with $h = 0.025$, the interval of integration is $[0, 500]$.

It has to be noted, that once again, the symmetric exponential integrator performs better than the other two schemes.

In Figure 3 and Figure 4 we plot the results for the conservative methods. In both experiments we integrated on the time interval $[0, 50]$, with time step $h = 0.025$, for the initial condition (18), and with $h = 0.0125$ for the initial condition (19). The experiments confirm

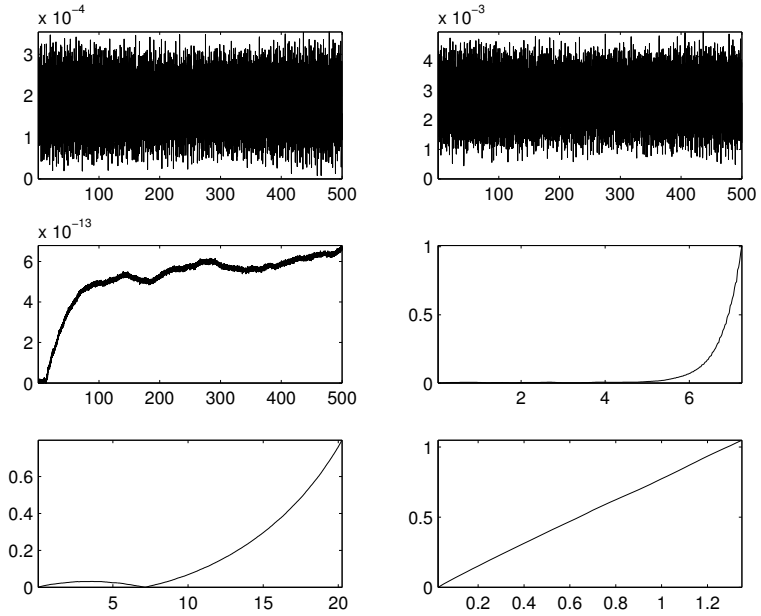


Figure 2: Density (left column) and energy along (SMEXP), (L1) and (PASSA) (from the top to the bottom) for the initial condition (19). Number of Fourier modes $M = 512$, time step 0.025.

the good conservation properties of the methods. In particular the method (SPMEXP-D) which performs the symmetric projection only for the density, conserves very well also the energy. In fact the error is about of the same size as the energy error obtained with the multisymplectic method (MULTI) and with the method (B).

Performing experiments with different sizes of M, the number of Fourier modes in the space discretization, and fixed time step $h = 0.025$, we also observed that the number of iterations needed to achieve convergence in the Newton iteration for the methods (SMEXP), (SPMEXP-D) and (SPMEXP-DE), remains nearly unchanged.

We have presented a new class of exponential integrators which have favourable geometric properties. The cost of this added quality is that the schemes are implicit in the nonlinear function $N(u)$. Each iteration needed for solving the resulting nonlinear system of equations costs approximately the same as a low order explicit exponential integrator. The number of iterations needed seems to depend only on the (local) Lipschitz constant of $N(u)$ and the stepsize, and not on the space discretization parameter. So far, tests have been conducted only with one stage schemes of order two, and only with the most common coefficient functions $a(z)$ and $b(z)$. The preliminary tests are promising, but it remains to try out and analyse schemes of higher order and to take advantage of the ample freedom available in choosing coefficient functions of the schemes.

References

[1] M. J. Ablowitz and J. F. Ladik. A nonlinear difference scheme and inverse scattering. *Studies in Appl. Math.*, 55(3):213–229, 1976.

[2] H. Berland, A. L. Islas, , and C. M. Schober. Conservation of phase space properties

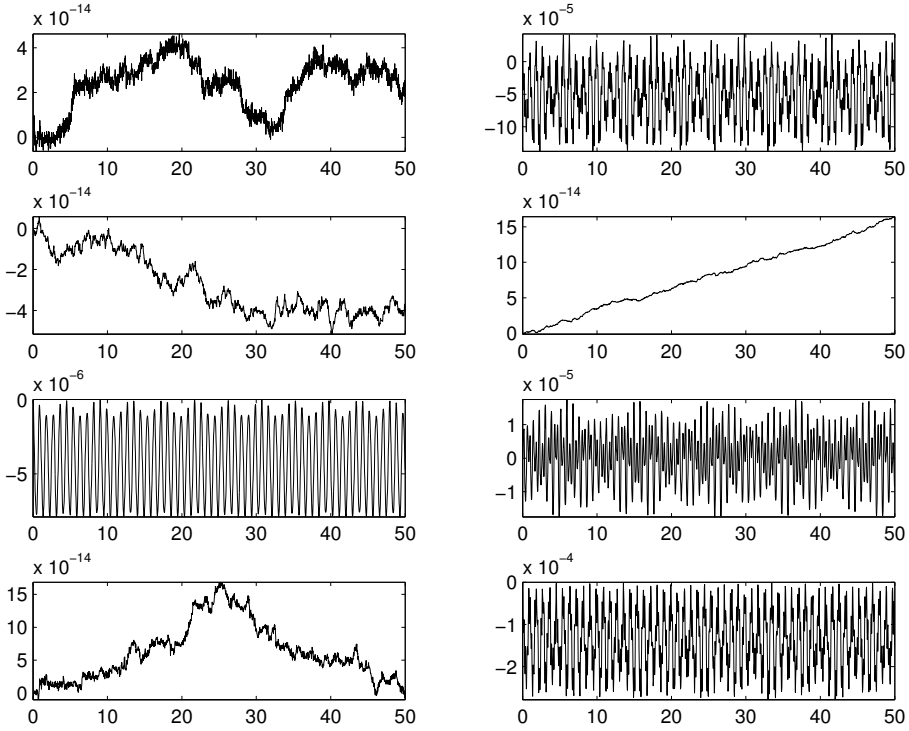


Figure 3: Density (left column) and energy along (SPMEXP-D), (SPMEXP-DE), (MULTI) and (B) (from the top to the bottom) for the initial condition (18). Number of Fourier modes $M = 512$, time step 0.025.

using exponential integrators on the cubic Schrödinger equation. Technical Report 1/06, Norwegian Institute of Science and Technology, 2006. submitted to J. Comp. Phys.

[3] H. Berland, B. Skaflestad, and W. M. Wright. EXPINT – a MATLAB package for exponential integrators. *ACM Transactions on Mathematical Software*, 33(1), March 2007.

[4] C. Besse. A relaxation scheme for the nonlinear Schrödinger equation. *SIAM J. Numer. Anal.*, 42(3):934–952 (electronic), 2004.

[5] T. J. Bridges and S. Reich. Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity. *Phys. Lett. A*, 284(4-5):184–193, 2001.

[6] B. Cano. Conserved quantities of some Hamiltonian wave equations after full discretization. *Numer. Math.*, 103(2):197–223, 2006.

[7] J. Certaine. The solution of ordinary differential equations with large time constants. In *Mathematical methods for digital computers*, pages 128–132. Wiley, New York, 1960.

[8] A. Durán and J. M. Sanz-Serna. The numerical integration of relative equilibrium solutions. The nonlinear Schrödinger equation. *IMA J. Numer. Anal.*, 20(2):235–261, 2000.

[9] Z. Fei, V. M. Pérez-García, and L. Vázquez. Numerical simulation of nonlinear Schrödinger systems: a new conservative scheme. *Appl. Math. Comput.*, 71(2-3):165–177, 1995.

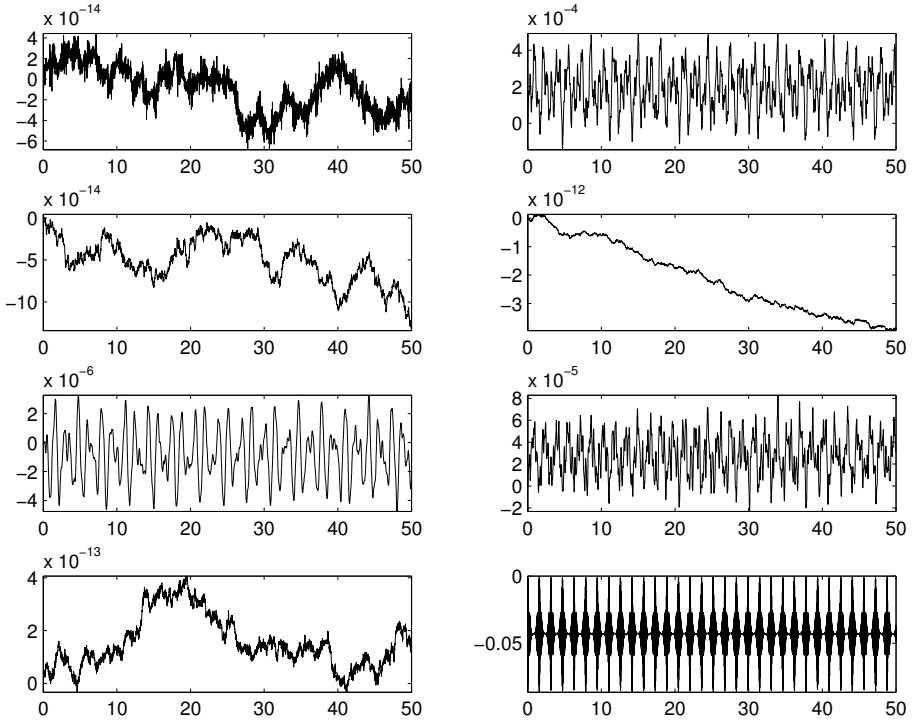


Figure 4: Density (left column) and energy along (SPMEXP-D), (SPMEXP-DE), (MULTI) and (B) (from the top to the bottom) for the initial condition (19). Number of Fourier modes $M = 512$, timestep 0.0125.

[10] E. Hairer. Symmetric projection methods for differential equations on manifolds. *BIT*, 40(4):726–734, 2000.

[11] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.

[12] A. L. Islas, D. A. Karpeev, and C. M. Schober. Geometric integrators for the nonlinear Schrödinger equation. *J. Comput. Phys.*, 173(1):116–148, 2001.

[13] A. L. Islas and C. M. Schober. On the preservation of phase space structure under multisymplectic discretization. *J. Comput. Phys.*, 197(2):585–609, 2004.

[14] J. D. Lawson. Generalized Runge-Kutta processes for stable systems with large Lipschitz constants. *SIAM J. Numer. Anal.*, 4:372–380, 1967.

[15] J. E. Marsden and T. S. Ratiu. *Introduction to mechanics and symmetry*, volume 17 of *Texts in Applied Mathematics*. Springer-Verlag, New York, second edition, 1999. A basic exposition of classical mechanical systems.

[16] R. I. McLachlan. Symplectic integration of Hamiltonian wave equations. *Numer. Math.*, 66(4):465–492, 1994.

[17] B. Minchev and W. M. Wright. A review of exponential integrators for semilinear problems. Technical Report 2/05, Department of Mathematical Sciences, NTNU, Norway, 2005. `http://www.math.ntnu.no/preprint/`.

[18] S. Reich. Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations. *J. Comput. Phys.*, 157(2):473–499, 2000.

[19] T. R. Taha and J. Ablowitz. Analytical and numerical aspects of certain nonlinear evolution equations. II. Numerical, nonlinear Schrödinger equation. *J. Comput. Phys.*, 55(2):203–230, 1984.

[20] A. Zanna, K. Engø, and H. Munthe-Kaas. Adjoint and selfadjoint Lie-group methods. *BIT*, 41(2):395–421, 2001.