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A Note on the Symplectic Integration of the Nonlinear Schrödinger Equation

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Abstract. Numerically solving the nonlinear Schrödinger equation and being able to treat arbitrary space dependent potentials permits many application in the realm of quantum mechanics. The long-term stability of a numerical method and its conservation properties is an important feature since it assures that the underlying physics of the solution are respected and it ensures that the numerical result is correct also for small time spans. In this paper we describe symplectic integrators for the nonlinear Schrödinger equation with arbitrary potentials and perform numerical experiments comparing different approaches and highlighting their respective advantages and disadvantages.

Keywords: nonlinear Schrödinger equations, symplectic integration, difference methods

1. Introduction

The motivation for considering the time-dependent Schrödinger equation and its solutions for large time spans stems from the fact that quantum-mechanical effects will play a dominating role in nano-scale semiconductor devices and in new device concepts beyond traditional CMOS based on silicon technology (e.g., single-electron devices and resonant-tunneling devices) [1]. Numerical schemes of this kind are also a prerequisite for the transient simulation of proposed devices like quantum dots and quantum cellular automata [2,3].

The wave equation or the time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V_0\cdot\psi(\mathbf{r},t)$$

describes the non-relativistic quantum mechanics for particles without spin. Here a particle of mass m moves in a field represented by the potential energy function V_0. Scaling this equation yields the equations considered in this work.

In the following we consider the Schrödinger equation in the form

$$\mathrm{i}u_t + u_{xx} + 2uV(t,x,u) = 0.$$

$V(t,x,u)$ denotes the potential and in the case of the Schrödinger equation with cubic nonlinearity in one space dimension it is of the form $V(t,x,u) = |u|^2 + V_1(t,x)$, where $V_1(t,x)$ is an arbitrary real valued function. More precisely, we are interested in numerical solutions of the initial boundary value problem

$$\begin{aligned}
&u:[0,T]\times[0,1]\to\mathbb{C}\\
&\mathrm{i}u_t + u_{xx} + 2uV(t,x,u) = 0\\
&u(0,x)\text{ given}\\
&\text{periodic boundary conditions for } x\in[0,1]
\end{aligned}$$

obtained by methods of geometric integration.

A review of the analytical properties of the solutions of the cubic nonlinear Schrödinger equation can be found in [4] which also discusses the connection of this PDE to dynamical systems. This nonlinear equation shows interesting phenomena like solitary waves and solitons, finite-time blow-up, chaotic evolution in deterministic PDEs, and periodic waves and quasi-periodic wave-trains. It also has applications to nonlinear optics, laser dynamics, and photonics [5,6]. Implementors of simulators for quantum dots and similar applications will be more interested in the equation with the linear potential term, to which the same methods can be applied in a straightforward manner.

Runge–Kutta methods and linear multi-step methods for ODEs have reached a high level of maturity and are generally available program codes. Although Runge–Kutta methods can conserve linear and quadratic invariants, no Runge–Kutta method can conserve all polynomial invariants of degree three and higher [7]. This motivates the search for new methods which respect the geometric properties of the solutions.

The main idea of the geometric integration of ODEs and PDEs is that the geometry of the equation to be solved should be respected by the numerical method, i.e., invariants of the equation are also conserved by the numerical integrator [7–10].

The method of Poisson integrators, a generalization of symplectic integrators, will be used to derive implicit finite difference schemes for the problem above. The paper is organized into an introduction to symplectic integrators for Hamiltonian systems in Section 2, a recapitulation of Poisson integrators and their application to the initial boundary value problem in Sections 3 and 4, and finally several numerical results for the nonlinear Schrödinger equation are presented in Section 5.

2. Symplectic Integrators

We start by defining the notion of symplectic (i.e., area preserving) functions. A linear function is defined to be symplectic if it conserves oriented area as defined by the parallelogram spanned by two vectors. Hence a differentiable function is called symplectic if its Jacobian is everywhere symplectic.

There is an interesting connection between symplectic functions and Hamiltonian systems, i.e., systems of the form

$$\begin{aligned} \dot{p} &= -\nabla_q H(p,q) \\ \dot{q} &= \nabla_p H(p,q), \end{aligned}$$

where p and q are vectors denoting momentum and position, respectively. $H(p,q)$ is the Hamiltonian and a first integral of the system. The following theorem is due to Poincaré [7,11].

Theorem 2.1. *Let $H(p,q)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$ defining a Hamiltonian system. Then the flow φ_t of the Hamiltonian system (i.e., the mapping that advances the solution by time) is a symplectic transformation (wherever it is defined) for all t.*

The converse is also true:

Theorem 2.2. *Let $f : U \to \mathbb{R}^{2d}$ be a continuously differentiable function. Then the system $\dot{y} = f(y)$ is locally Hamiltonian (i.e., it can locally be written in the form of a Hamiltonian system) if and only if its flow $\varphi_t(y)$ is symplectic for all $y \in U$ and for all sufficiently small t.*

Because of the characteristic symplectic nature of the flow of a Hamiltonian system, it is natural to search for numerical methods sharing this property. Hence we extend the definition of symplecticity to numerical one-step methods.

Definition 2.3. A numerical one-step method is called *symplectic*, if the one-step map $y_{n+1} = \Phi_h(y_n)$ is symplectic whenever the method is applied to a smooth Hamiltonian system.

Examples of symplectic one-step methods are the symplectic Euler scheme

$$\begin{aligned} p_{n+1} &= p_n - h\frac{\partial H}{\partial q}(p_{n+1}, q_n) \\ q_{n+1} &= q_n + h\frac{\partial H}{\partial p}(p_{n+1}, q_n) \end{aligned}$$

which is of order 1. The same holds for its adjoint method

$$\begin{aligned} p_{n+1} &= p_n - h\frac{\partial H}{\partial q}(p_n, q_{n+1}) \\ q_{n+1} &= q_n + h\frac{\partial H}{\partial p}(p_n, q_{n+1}). \end{aligned}$$

The implicit mid-point rule

$$\begin{aligned} p_{n+1} &= p_n - h\frac{\partial H}{\partial q}\big((p_{n+1}+p_n)/2, (q_{n+1}+q_n)/2\big) \\ q_{n+1} &= q_n + h\frac{\partial H}{\partial p}\big((p_{n+1}+p_n)/2, (q_{n+1}+q_n)/2\big) \end{aligned}$$

is a symplectic method of order 2. Furthermore compositions of symplectic methods are again symplectic methods, which is one way to construct higher-order symplectic schemes.

Examples of symplectic Gauss collocation (or Runge–Kutta) methods are the following. If s is the degree of the collocation polynomial, then the Gauss

Table 1. Butcher tableaus of Gauss collocation methods of order 4 and 6.

$1/2-\sqrt{3}/6$	$1/4$	$1/4-\sqrt{3}/6$
$1/2+\sqrt{3}/6$	$1/4+\sqrt{3}/6$	$1/4$
	$1/2$	$1/2$

$1/2-\sqrt{15}/10$	$5/36$	$2/9-\sqrt{15}/15$	$5/36-\sqrt{15}/30$
$1/2$	$5/36+\sqrt{15}/24$	$2/9$	$5/36-\sqrt{15}/24$
$1/2+\sqrt{15}/10$	$5/36+\sqrt{15}/30$	$2/9+\sqrt{15}/15$	$5/36$
	$5/18$	$4/9$	$5/18$

collocation methods are of order $2s$. For $s=1$ we again have the implicit midpoint rule

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}, \tag{1}$$

and the methods for $s=2$ (order 4) and $s=3$ (order 6) are shown in Table 1.

The conservation property of symplectic methods is condensed in the following important result obtained by backward error analysis [7,12]. After truncation, the modified Hamiltonian is

$$\tilde{H}(y) = H(y) + h^m H_{m+1}(y) + \cdots + h^{N-1} H_N(y),$$

where m is the order of the method.

Theorem 2.4 (*Long Term Energy Conservation*). *If a symplectic numerical method of order m with step size h is applied to a Hamiltonian system with analytic $H: D \to \mathbb{R}$ (where $D \subset \mathbb{R}^{2d}$) and the numerical solution remains in a compact set $K \subset D$, then there are h_0 and $N(h)$ such that*

$$\begin{aligned} \tilde{H}(y_n) &= \tilde{H}(y_0) + O(\mathrm{e}^{-h_0/2h}) \\ H(y_n) &= H(y_0) + O(h^m) \end{aligned}$$

over exponentially long time intervals $nh \le \mathrm{e}^{h_0/2h}$.

It is one of the favorable properties of symplectic methods that these equations hold for exponentially long time intervals. For a non-symplectic method the second equation would generally read $H(y_n) = H(y_0) + O(nh^m)$ meaning that the error would generally increase linearly with time.

3. Poisson Integrators

Unfortunately many systems of practical importance, especially those for quantum-mechanical systems, cannot be written as Hamiltonian systems. Generalizing the ideas from Section 2 to systems of the form

$$\dot{y} = P(y)\nabla H(y), \tag{2}$$

where $P(y)$ is a Poisson bracket, leads to Poisson integrators. In the previous section we had $y=(p,q)$ and $P(y) = J^{-1}$, where

$$J := \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{3}$$

and I is the identity matrix. In this section we summarize the generalization to more general $P(y)$. It is based on the Darboux–Lie Theorem and hence classic work by Clebsch, Darboux, Jacobi, and Lie [7, 13–16].

We start with some definitions.

Definition 3.1 (Poisson Bracket). Let $P(y) = p_{ij}(y)$ $(i, j \in \{1, \ldots, n\})$ be a smooth matrix-valued function. If

$$\begin{aligned} \{F, G\}(y) &:= \nabla F(y)^T P(y) \nabla G(y) \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial F(y)}{\partial y_i} p_{ij}(y) \frac{\partial G(y)}{\partial y_j} \end{aligned}$$

is bilinear, skew-symmetric ($\{F, G\} = -\{G, F\}$), and satisfies Leibniz's rule

$$\{F \cdot G, H\} = F \cdot \{G, H\} + G \cdot \{F, H\}$$

and the Jacobi identity

$$\big\{\{F, G\}, H\big\} + \big\{\{H, F\}, G\big\} + \big\{\{G, H\}, F\big\} = 0$$

for sufficiently smooth F, G, and H, then $\{F, G\}(y)$ is called the Poisson bracket of F and G.

Definition 3.2 (Poisson System). If $P(y)$ represents a Poisson bracket, then

$$\dot{y} = P(y)\nabla H(y)$$

is called a Poisson system. Again H is called the Hamiltonian.

Lemma 3.3. *$P(y)$ represents a Poisson bracket if and only if $P(y)$ is a skew-symmetric matrix and the condition $\forall\forall\forall i, j, k$:*

$$\sum_{\nu=1}^{n} \left(\frac{\partial p_{ij}(y)}{\partial y_\nu} p_{\nu k}(y) + \frac{\partial p_{jk}(y)}{\partial y_\nu} p_{\nu i}(y) + \frac{\partial p_{ki}(y)}{\partial y_\nu} p_{\nu j}(y) \right) = 0$$

for the Jacobi identity is satisfied. (*Because of the structure of the Poisson bracket as a sum it is always bilinear and and always satisfies Leibniz's rule.*)

It is trivial to check that J defined in (3) indeed represents a Poisson bracket.

The Darboux–Lie Theorem answers the question which coordinate transformation of a Poisson system yields the simplest possible form—or canonical form—of $P(y)$.

Definition 3.4 (Canonical Form). A Poisson system represented by $P(y)$ is said to be in canonical form if it is of the form

$$P(y) = \begin{pmatrix} J^{-1} & 0 \\ 0 & 0 \end{pmatrix}.$$

Theorem 3.5 (*Darboux–Lie*). *Let $P(y)$ represent a Poisson system. If $P(y)$ is of constant rank $n - r = 2m$ in a neighborhood of $y_0 \in \mathbb{R}^n$, then there are functions $P_1(y), \ldots, P_m(y)$, $Q_1(y), \ldots, Q_m(y)$, and (the so-called Casimirs) $C_1(y), \ldots, C_r(y)$ so that*

$$\begin{array}{lll} \{P_i, P_j\} = 0 & \{P_i, Q_j\} = -\delta_{ij} & \{P_i, C_l\} = 0 \\ \{Q_i, P_j\} = \delta_{ij} & \{Q_i, Q_j\} = 0 & \{Q_i, C_l\} = 0 \\ \{C_k, P_j\} = 0 & \{C_k, Q_j\} = 0 & \{C_k, C_l\} = 0 \end{array}$$

holds in a neighborhood of y_0. The gradients of P_i, Q_i, and C_k are linearly independent and hence $y \mapsto (P_i(y), Q_i(y), C_k(y))$ is a local change of coordinates to canonical form.

The proof is constructive and, roughly speaking, works by iterating over the rows and columns of the structure matrix to find suitable coordinates P_i and Q_i as solutions of linear PDEs.

Important properties of Hamiltonian systems are also true for Poisson systems. First the Hamiltonian of the Poisson system is again a first integral. Analogously to symplectic maps, it is possible to define Poisson maps. Then in analogy to Theorem 2.1 it can be proven under certain smoothness assumptions that a system is locally a Poisson system, whose structure matrix is a Poisson bracket, if and only if its flow is a Poisson map and respects the Casimirs of the transformation of the Poisson bracket to canonical form. Again, as in the case of Definition 2.3, this motivates the following definition.

Definition 3.6. A numerical one-step method is called a *Poisson integrator* for a Poisson system with structure matrix $P(y)$, if the one-step map $y_{n+1} = \Phi_h(y_n)$ is a Poisson map whenever it is applied to the Poisson system and if Φ_h respects the Casimirs of the transformation of $P(y)$ to canonical form.

Clearly a numeric integrator can only be a Poisson integrator for certain structure matrices $P(y)$.

Table 2 summarizes how the concepts for Hamiltonian systems, i.e., systems with canonical Poisson bracket, and systems with general Poisson bracket relate to one another. These considerations give rise to a Poisson integrator for Poisson systems. In summary it consists of the following steps:

1. First find the transformation $\varphi(y) := (P_i(y), Q_i(y), C_k(y))$ to canonical form for the given structure matrix $P(y)$ by using Theorem 3.5.

Table 2. The column on the left hand side lists some concepts for Hamiltonian systems and the corresponding concepts for general Poisson systems are shown on the right hand side. The transformation to canonical Poisson form allows to translate between these two.

Hamiltonian system	Poisson system
Canonical form	General Poisson bracket
Symplectic transformation	Poisson map
Flow is symplectic	Flow is a Poisson map and respects the Casimirs
Symplectic integrator	Poisson integrator

2. Define $z_n := \varphi(y_n)$ and apply a symplectic integrator to the transformed system which has now a structure matrix in canonical form (cf. Definition 3.4).
3. Transform back to the original coordinates $y_n = \varphi^{-1}(z_n)$.

4. Poisson Integrators for the Nonlinear Schrödinger Equation

We now carry out the ideas of the previous sections for the nonlinear equation in its most general form

$$\mathrm{i}u_t + u_{xx} + 2\alpha u(|u|^2 + V_1(t,x)) = 0$$

for periodic boundary conditions. V_1 is a real valued function and $\alpha \in \mathbb{R}\backslash\{0\}$. Depending on how the nonlinear term is discretized, one can write the system in Hamiltonian form in straightforward manner ($u \mapsto w_k$, Section 4.1) or one arrives at the Ablowitz–Ladik model ($2u \mapsto w_{k-1} + w_{k+1}$, Section 4.2).

4.1. A Hamiltonian for the Canonical Form

Discretizing the derivations with respect to the space variable first in an equidistant manner, we obtain the equations

$$\mathrm{i}\frac{\partial w_k}{\partial t} + \frac{w_{k+1} - 2w_k + w_{k-1}}{\Delta x^2} + 2\alpha w_k(|w_k|^2 + V_1(t,x)) = 0$$

in the new variables $w_k, k \in \{1,\dots,N\}$. In the next step we split the new variables w_k into real and imaginary parts via $w_k = u_k + \mathrm{i}v_k$. This yields

$$\begin{aligned}\frac{\partial u_k}{\partial t} &= -\frac{1}{\Delta x^2}(v_{k+1} - 2v_k + v_{k-1}) \\ &\quad - 2\alpha v_k\big(u_k^2 + v_k^2 + V_1(t,x)\big) \\ \frac{\partial v_k}{\partial t} &= \frac{1}{\Delta x^2}(u_{k+1} - 2u_k + u_{k-1}) \\ &\quad + 2\alpha u_k\big(u_k^2 + v_k^2 + V_1(t,x)\big).\end{aligned}$$

Introducing the notation $u := (u_1,\dots,u_N)$ and $v := (v_1,\dots,v_N)$ and defining the Hamiltonian

$$H(u,v) := \frac{1}{\Delta x^2}\sum_{k=1}^{N}\big(u_k u_{k-1} - u_k^2 + v_k v_{k-1} - v_k^2\big) + \frac{\alpha}{2}\sum_{k=1}^{N}\big(u_k^2 + v_k^2 + V_1(t,x)\big)^2$$

we obtain

$$\begin{pmatrix}\dot u \\ \dot v\end{pmatrix} = \begin{pmatrix}0 & -I \\ I & 0\end{pmatrix}\begin{pmatrix}\nabla_u H(u,v) \\ \nabla_v H(u,v)\end{pmatrix},$$

and have thus written the system in canonical form.

4.2. A Transformation for the Ablowitz–Ladik Model

To arrive at the Ablowitz-Ladik model, we now discretize the nonlinear term using $2u \mapsto w_{k-1} + w_{k+1}$ [17, 18] and obtain

$$\mathrm{i}\frac{\partial w_k}{\partial t} + \frac{w_{k+1} - 2w_k + w_{k-1}}{\Delta x^2} + \alpha(w_{k-1} + w_{k+1})(|w_k|^2 + V_1(t,x)) = 0$$

in the new variables w_k, $k \in \{1,\dots,N\}$. Again we split the new variables w_k into real and imaginary parts via $w_k = u_k + \mathrm{i}v_k$. This yields

$$\begin{aligned}\frac{\partial u_k}{\partial t} &= -\frac{1}{\Delta x^2}(v_{k+1} - 2v_k + v_{k-1}) \\ &\quad - \alpha(v_{k+1} + v_{k-1})\big(u_k^2 + v_k^2 + V_1(t,x)\big) \\ \frac{\partial v_k}{\partial t} &= \frac{1}{\Delta x^2}(u_{k+1} - 2u_k + u_{k-1}) \\ &\quad + \alpha(u_{k+1} + u_{k-1})\big(u_k^2 + v_k^2 + V_1(t,x)\big).\end{aligned}$$

We can write these equations in the form of (2). Introducing the notation $u := (u_1,\dots,u_N)$ and $v := (v_1,\dots,v_N)$ we obtain

$$\begin{pmatrix}\dot u \\ \dot v\end{pmatrix} = \begin{pmatrix}0 & -D \\ D & 0\end{pmatrix}\begin{pmatrix}\nabla_u H(u,v) \\ \nabla_v H(u,v)\end{pmatrix},$$

where the entries of the diagonal matrix D are

$$d_k := 1 + \alpha\Delta x^2\big(u_k^2 + v_k^2 + V_1(t,x)\big)$$

and

$$H(u,v) := \frac{1}{\Delta x^2}\sum_{k=1}^{N}(u_k u_{k-1} + v_k v_{k-1}) - \frac{1}{\alpha\Delta x^4} \times \sum_{k=1}^{N}\ln\big(1 + \alpha\Delta x^2\big(u_k^2 + v_k^2 + V_1(t,x)\big)\big).$$

Checking the conditions from Definition 3.1 via Lemma 3.3 is straightforward. (This is in fact true for

all systems where $P(y)$ has the structure

$$P(y) = \begin{pmatrix} 0 & -D \\ D & 0 \end{pmatrix} \tag{4}$$

with D being a diagonal matrix.) Fortunately this system is a Poisson system (Definition 3.2) and the theory of Section 3 can be applied.

The transformation to canonical form is not unique and will generally depend on V_1, since d_k depends on V_1. However, the transformation to canonical form should be global, i.e., it should be identical for all time steps; otherwise poor performance as time progresses has to be expected [7]. Therefore we assume in the following that $V_1(t, x)$ vanishes.

In order to find a transformation to canonical form, we have to employ Theorem 3.5 and set $y := (p_1, \ldots, p_N, q_1, \ldots, q_N)$. For our $P(y)$, the conventional procedure is to define $Q_1(y) := y_1$ and solve the linear PDE$\{Q_1, P_1\} = 1$. This yields the transformation given in [19] for a transformed Schrödinger equation, which does not treat the variables u and v symmetrically.

Because of $d_k(u, v) = d_k(v, u)$ and $H(u, v) = H(v, u)$ it is desirable to find a transformation so that the relations $p_k(u, v) = p_k(v, u)$ and $q_k(u, v) = q_k(v, u)$ hold for the new variables p_k and q_k . We also use the ansatz $P_1 = P_1(y_1, y_{N+1})$ and $Q_1 = Q_1(y_1, y_{N+1})$ which is equivalent to $p_k = p_k(u_k, v_k)$ and $q_k = q_k(u_k, v_k)$. Due to the special structure (4) of $P(y)$, we have $r = 0$ in Theorem 3.5 and it can be verified that are the conditions $\{P_i, P_j\} = 0$ and $\{Q_i, Q_j\} = 0$ of Theorem 3.5 are always fulfilled for structure matrices of this form. Therefore we have to find symmetric solutions of $\{Q_1, P_1\} = 1$ which is equivalent to

$$\begin{aligned} -\frac{\partial Q_1}{\partial y_1}\frac{\partial P_1}{\partial y_{N+1}} + \frac{\partial Q_1}{\partial y_{N+1}}\frac{\partial P_1}{\partial y_1} &= \frac{1}{d_k} \\ &= \frac{1}{1 + \alpha\Delta x^2\left(y_1^2 + y_{N+1}^2\right)}. \end{aligned}$$

The right hand side suggests the substitution $z := \alpha\Delta x^2(y_1^2 + y_{N+1}^2)$. The simple ansatz $P_1 = y_1\sigma(z)$ and $Q_1 = y_{N+1}\sigma(z)$ leads to the ODE

$$\sigma^2 + 2z\sigma\sigma' = \frac{1}{1+z}$$

which has the solution

$$\sigma(x) := \sqrt{\frac{\ln(1+x)}{x}}.$$

Hence we arrive at the transformation

$$\begin{aligned} p_k &:= u_k\sigma\left(\alpha\Delta x^2\left(u_k^2 + v_k^2\right)\right) \\ q_k &:= v_k\sigma\left(\alpha\Delta x^2\left(u_k^2 + v_k^2\right)\right), \end{aligned}$$

which was also proposed in [7]. Its inverse transformation is

$$\begin{aligned} u_k &= p_k\tau\left(\alpha\Delta x^2\left(p_k^2 + q_k^2\right)\right) \\ v_k &= q_k\tau\left(\alpha\Delta x^2\left(p_k^2 + q_k^2\right)\right), \end{aligned}$$

where

$$\tau(x) := \sqrt{\frac{\mathrm{e}^x - 1}{x}}.$$

The inverse is found by observing that

$$\alpha\Delta x^2\left(p_k^2 + q_k^2\right) = \ln\left(1 + \alpha\Delta x^2\left(u_k^2 + v_k^2\right)\right)$$

and

$$\mathrm{e}^{\alpha\Delta x^2\left(p_k^2+q_k^2\right)} - 1 = \alpha\Delta x^2\left(u_k^2 + v_k^2\right),$$

which leads to

$$\frac{\mathrm{e}^{\alpha\Delta x^2\left(p_k^2+q_k^2\right)} - 1}{\alpha\Delta x^2\left(p_k^2 + q_k^2\right)^2} = \frac{\alpha\Delta x^2\left(u_k^2 + v_k^2\right)}{\ln\left(1 + \alpha\Delta x^2\left(u_k^2 + v_k^2\right)\right)}$$

and thus

$$\tau\left(\alpha\Delta x^2\left(p_k^2 + q_k^2\right)\right) = \frac{1}{\sigma\left(\alpha\Delta x^2\left(u_k^2 + v_k^2\right)\right)}.$$

Therefore we have $u_k = p_k/\sigma(\alpha\Delta x^2(u_k^2 + v_k^2)) = p_k\tau(\alpha\Delta x^2(p_k^2 + q_k^2))$ and analogously $v_k = q_k/\sigma(\alpha\Delta x^2(u_k^2 + v_k^2)) = q_k\tau(\alpha\Delta x^2(p_k^2 + q_k^2))$.

After the transformation the new Hamiltonian H in the variables p and q reads

$$\begin{aligned} H(p, q) = \frac{1}{\Delta x^2}\sum_{k=1}^{N} &\tau\left(\alpha\Delta x^2\left(p_k^2 + q_k^2\right)\right) \\ &\times \tau\left(\alpha\Delta x^2\left(p_{k-1}^2 + q_{k-1}^2\right)\right) \\ &\times (p_k p_{k-1} + q_k q_{k-1}) \\ &- \frac{1}{\alpha\Delta x^4}\sum_{k=1}^{N} \ln\left(\mathrm{e}^{\alpha\Delta x^2\left(p_k^2+q_k^2\right)}\right. \\ &\left. + \alpha\Delta x^2 V_1(t, x)\right). \end{aligned}$$

Symplectic schemes can now be applied to this Hamiltonian as described in Section 3.

5. Numerical Results

We use the numeric integrators to simulate physical situations of interest. The first example is a recurrence similar to those recently observed in optical fibers. The second one is a soliton hitting a sidewall potential. In the first example we compare the two Hamiltonian based methods from Section 4.

The symplectic methods from Section 2 are implicit. In the following examples experience showed that fixed-point iteration yields much better results than Newton methods, and hence fixed-point iteration was used to obtain all of the numerical results.

5.1. A Recurrence

Recently, an optical Fermi–Pasta–Ulam recurrence [20] was demonstrated experimentally in an optical fiber [5,6]. In this example we consider the equation with $\alpha := 1$. We start from the initial condition $u(0, x) := \pi\sqrt{2}(1 + \frac{1}{10}\cos(\pi x))$ and use periodic boundary conditions for $x \in [-1, 1]$. The symplectic scheme for solving the ODEis the sixth order Gauss collocation method (Table 1) and $N := 50$.

Using the scheme from Section 4.1 we obtain the solution shown in Fig. 1. The value of the mass varies between approximately 39.675809692379175 and 39.67580969237926 and is well-conserved. The same is true for the Hamiltonian from Section 4.1, which varies between approximately 10009.181417277767 and 10009.18141727789.

The scheme from Section 4.2 results in the solution shown in Fig. 2. The notable variation in mass is shown in Fig. 3. The Hamiltonian from Section 4.2 is well-conserved and stays between approximately 9793.991350824712 and 9793.99135082576.

For reference Fig. 4 shows the solution found by a first-same-as-last embedded pair of explicit Runge–Kutta methods of order 6 using automatic time-step control. The notable variation in mass is shown in Fig. 5. The Hamiltonian (Section 4.2) is well-conserved and lies between approximately 9793.989394666394 and 9793.991573444684.

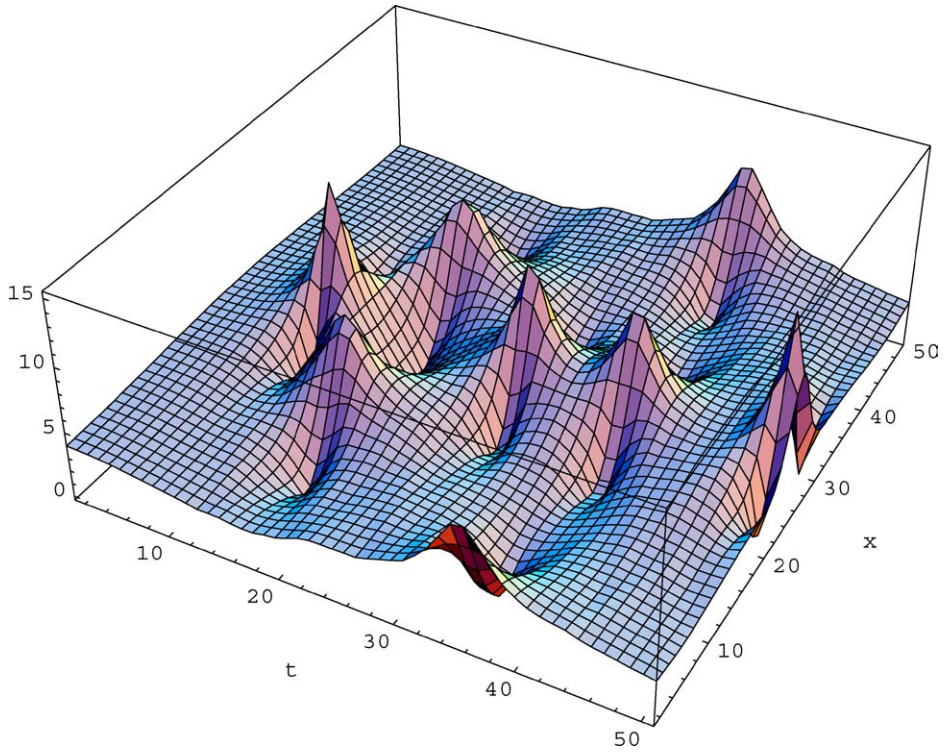

Figure 1. The absolute value of the solution found using the direct method for $t \in [0, 1]$ and $\Delta t := 5 \cdot 10^{-6}$.

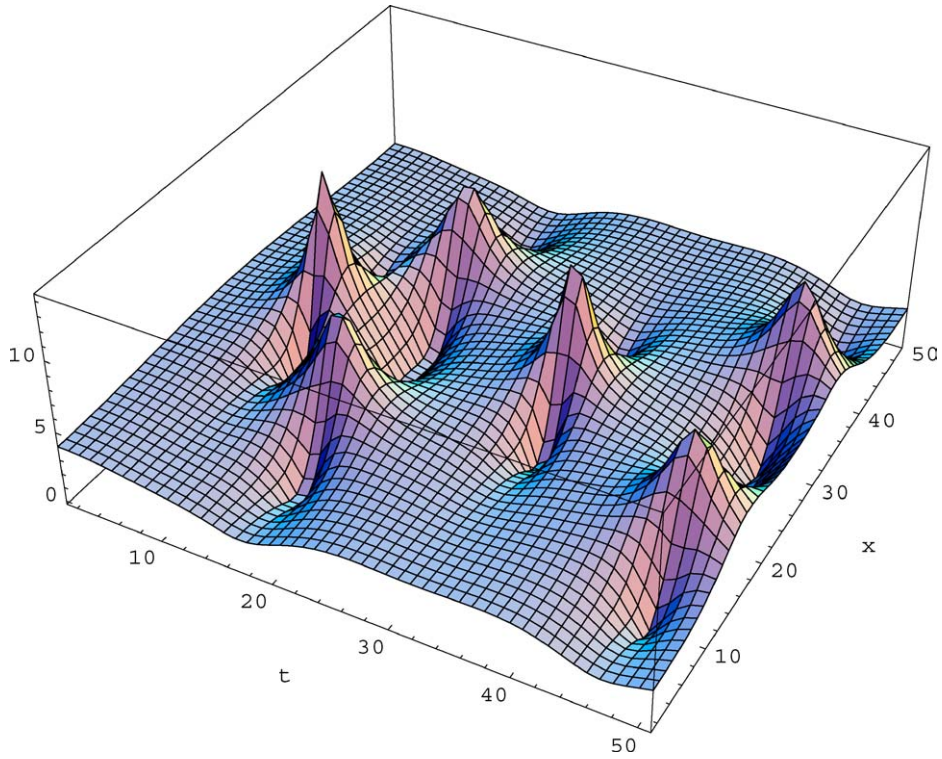

Figure 2. The absolute value of the solution found using the transformation to canonical form for $t \in [0, 1/2]$ and $\Delta t := 5 \cdot 10^{-6}$.

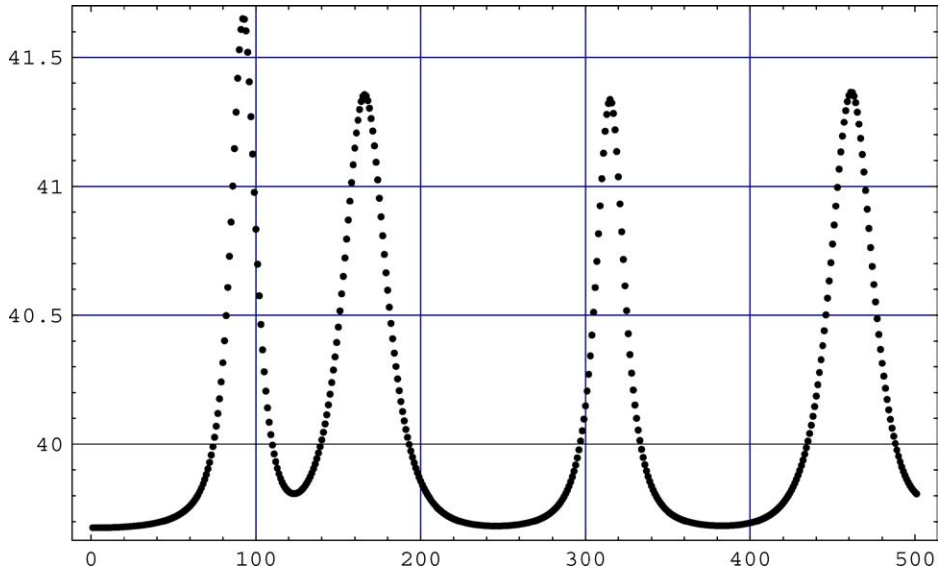

Figure 3. The variation in mass for $t \in [0, 1/2]$ for the solution shown in Fig. 2.

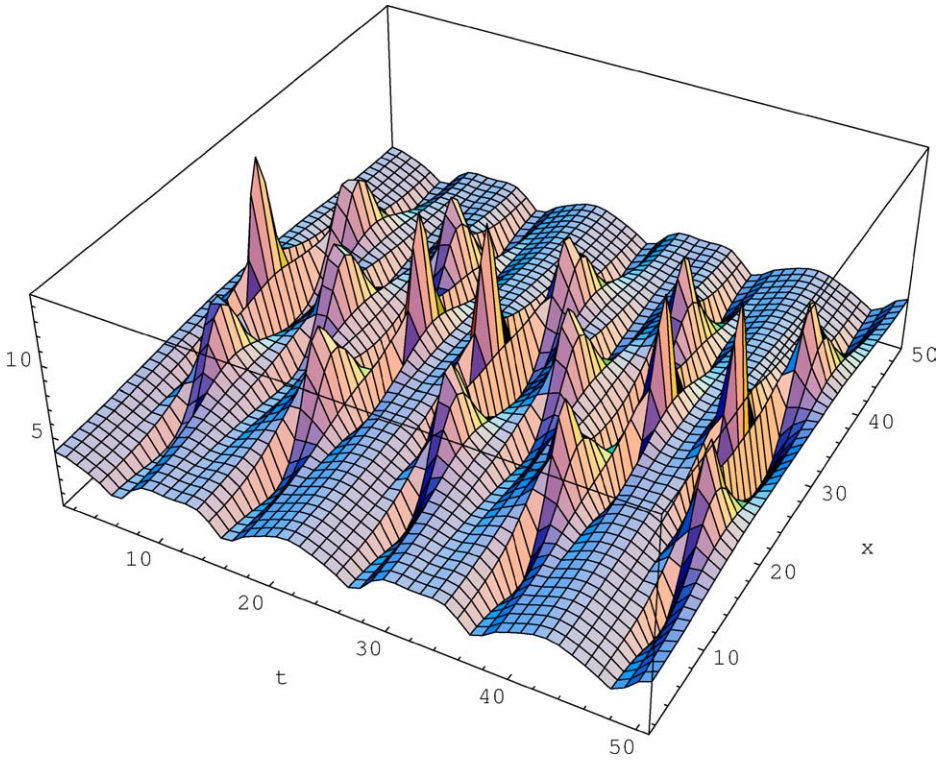

Figure 4. The absolute value of the solution found using a nonsymplectic scheme for $t \in [0, 3/2]$.

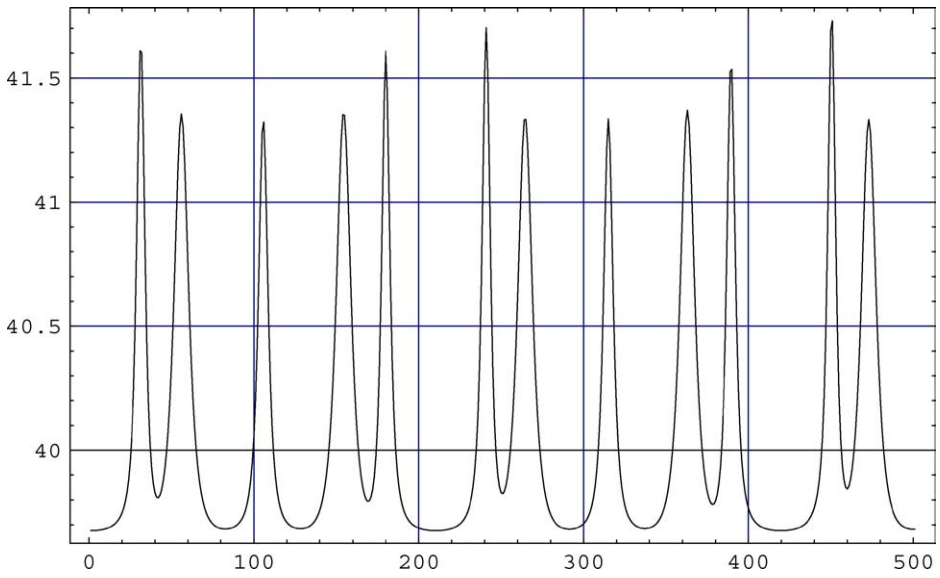

Figure 5. The variation in mass for $t \in [0, 3/2]$ for the solution shown in Fig. 4.

The analytic solution is unstable. The smallest perturbations result in large differences and this explains why the two solutions obtained from the two symplectic schemes (Figs. 1 and 2) show different behavior. Interestingly, mass is not conserved by the scheme from Section 4.2 as illustrated in Fig. 3.

5.2. *A Soliton Hitting a Sidewall Potential*

In this section we consider the nonlinear Schrödinger equation with $\alpha := 1/2$. Then a family of soliton solutions for $x \in \mathbb{R}$ is given by

$$u(t, x) := \beta \operatorname{sech} \frac{\beta(x - ct)}{\sqrt{2}} \mathrm{e}^{\mathrm{i}c(x-ct)/2+\mathrm{i}\gamma t},$$

where $c \in \mathbb{R}$ is the speed of the soliton and $\gamma \in \mathbb{R}$ a parameter so that $\beta^2 := 2(\gamma - c^2/4)$ has a positive solution for β.

In this example we chose $V(x) := 1000 \cdot \text{Heaviside}(x - 5)$ as the outside potential, $x \in [-5, 10]$, $N := 100$, and $\Delta t := 1/2000$. In total 40 000 time steps were performed for $t \in [0, 20]$. For solving the ODEwe used the sixth order Gauss collocation method (Table 1). The soliton is given by $c := 1/2$ and $\gamma := 10$.

Table 3. The mass during the solution shown in Figs. 6 and 7.

t	$M_{\text{symplectic}}(t)$	$M_{\text{non-symplectic}}(t)$
0	12.609519759413226	12.609519759413226
1	12.609519759413207	12.60951975931592
2	12.60951975941322	12.609519757302492
3	12.609519759413228	12.609519758590878
4	12.60951975941322	12.609519759345906
5	12.609519759413214	12.609519757434894
6	12.609519759413224	12.609519758628501
7	12.60951975941322	12.609519758122492
8	12.60951975941322	12.609519758026519
9	12.609519759413208	12.609519757267089
10	12.609519759413217	12.60951975749231
11	12.609519759413233	12.609519757496281
12	12.60951975941322	12.60951975766336
13	12.609519759413217	12.609519757865685
14	12.609519759413228	12.609519757582799
15	12.609519759413223	12.60951975899348
16	12.609519759413224	12.609519758558559
17	12.609519759413223	12.609519759362419
18	12.609519759413214	12.609519759412708
19	12.609519759413216	12.609519758967746
20	12.60951975941322	12.609519759415354

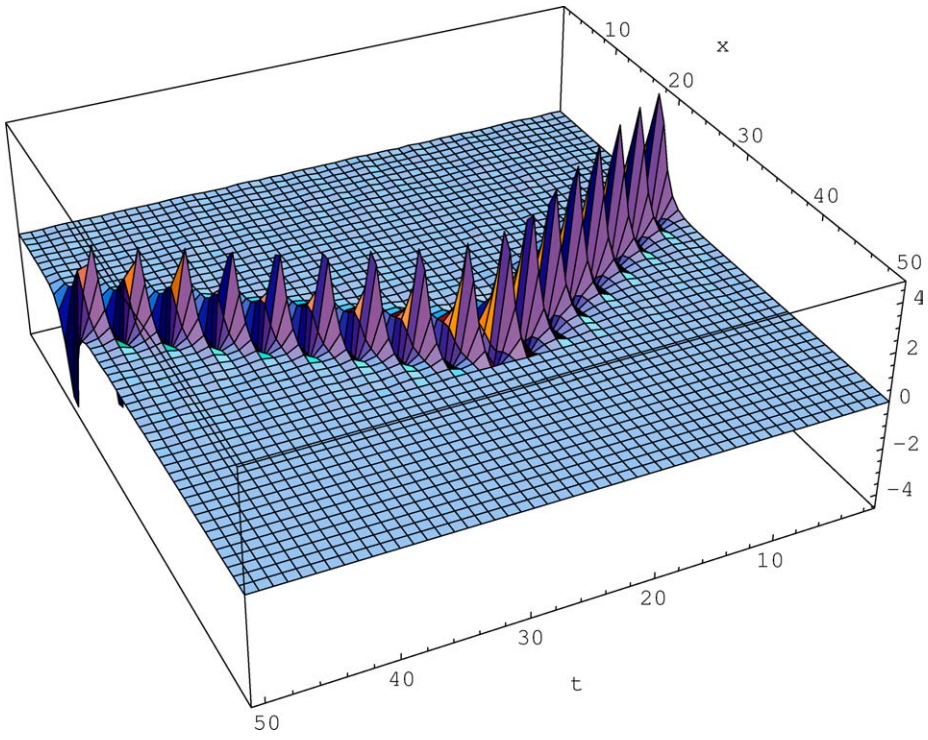

Figure 6. The real part, i.e., $u(t, x)$, of a soliton being reflected by a sidewall potential.

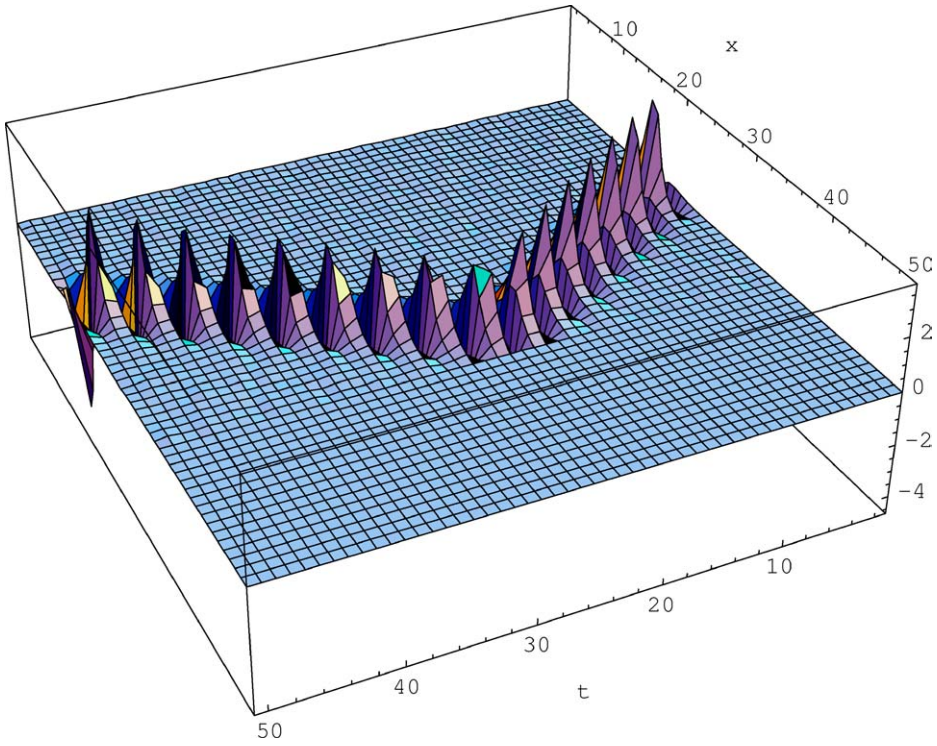

Figure 7. The imaginary part, i.e., $v(t, x)$, of a soliton being reflected by a sidewall potential.

Figures 6 and 7 show the real and imaginary part of the solution, respectively, as found by the scheme from Section 4.1. The scheme from Section 4.2 is not applicable, since the transformation to canonical Poisson form is not possible where the initial conditions are sufficiently close to zero.

Table 3 compares mass conservation using double-precision floating point numbers (about 16 digits). The mass difference between initial and final time step is $M_{\text{symplectic}}(20) - M(0) \approx -7.1 \cdot 10^{-15}$.

The second column shows the mass of several time steps of a solution obtained by a first-same-as-last embedded pair of explicit Runge–Kutta methods of order 6 using automatic time-step control. The change in mass is considerable.

6. Conclusion

Symplectic numerical methods are interesting because of their conservation properties and their long-term stability for exponentially long time spans. When applying these methods to PDEs, it is however not obvious how to write the ODE system obtained by the method of lines as a Hamiltonian system. It may not be possible to write it as a Hamiltonian system or the form as a Hamiltonian or Poisson system is not unique. Furthermore in the case of a Poisson system, the choice of the transformation to canonical form may influence the numerical results as well.

Symplectic numerical schemes were given for the nonlinear Schrödinger equation with a cubic nonlinearity. The nonlinear term of the equation may contain a arbitrary space and time dependent potential.

As the numerical experiments in Section 5 for the cubic nonlinear Schrödinger equation show, a mass conserving scheme is not necessarily obtained in this way. Examples for different behaviors are given and each of the numeric integrators has its respective advantages and disadvantages when considering computation time, accuracy, and conservation properties.

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