*International Journal of Computer Mathematics*
Vol. 00, No. 00, Month 200x, 1–22

# On multisymplecticity of partitioned Runge–Kutta and splitting methods

BRETT N. RYLAND*†, ROBERT I. MCLACHLAN† and JASON FRANK‡

†Institute of Fundamental Sciences, Massey University, Palmerston North, New Zealand

‡Center for Mathematics and Computer Science (CWI), P.O. Box 94079, 1090 GB Amsterdam, The Netherlands

(*XXXX*)

Although Runge–Kutta and partitioned Runge–Kutta methods are known to formally satisfy discrete multisymplectic conservation laws when applied to multi-Hamiltonian PDEs, they do not always lead to well-defined numerical methods. We consider the case study of the nonlinear Schrödinger equation in detail, for which the previously known multisymplectic integrators are fully implicit and based on the (second order) box scheme, and construct well-defined, explicit integrators, of various orders, with local discrete multisymplectic conservation laws, based on partitioned Runge–Kutta methods. We also show that two popular explicit splitting methods are multisymplectic.

*Keywords*: Multisymplectic; Multi-Hamiltonian; Runge–Kutta methods; Splitting methods; Nonlinear Schrödinger equation

*AMS Subject Classification*: 65M06; 65P10; 70S05

## 1. Introduction

Symplecticity is a property of Hamiltonian ODEs that has received a lot of attention in recent years due to the ability of symplectic integrators to accurately preserve the long-time behaviour of solutions of these ODEs. In particular, quasi-periodic orbits (KAM tori) and chaotic regions of phase space are preserved. The most popular symplectic integrators are explicit integrators based on splitting and implicit integrators based on Runge–Kutta [1, 2].

Along a solution of a Hamiltonian ODE ($\mathbf{K}z_t = \nabla_z S(z)$ where $z(t) \in \mathbb{R}^n$, $\mathbf{K}$ is skew symmetric and $S(z)$ is smooth), the variational equation associated with this ODE satisfies conservation of symplecticity, i.e.

$$\omega_t = 0, \tag{1}$$

where $\omega = \frac{1}{2}\mathbf{K}\mathrm{d}z \wedge \mathrm{d}z$ is the symplectic 2-form. A symplectic integrator preserves the integrated form of Eq. (1), namely $\omega^{n+1} = \omega^n$. A consequence of preserving this 2-form is that many first integrals of the system (most notably, energy) are approximately preserved by the integrator.

Multisymplecticity is the extension of symplecticity to Hamiltonian PDEs. We consider here PDEs that can be written in the multi-Hamiltonian form [3]

$$\mathbf{K}z_t + \mathbf{L}z_x = \nabla_z S(z), \tag{2}$$

where $z(t, x) \in \mathbb{R}^n$, $\mathbf{K}$ and $\mathbf{L}$ are skew-symmetric matrices and $S(z)$ is a smooth function. Along solutions $z(t, x)$ to a PDE of this form, the multisymplectic conservation law (MSCL)

$$\omega_t + \kappa_x = 0, \tag{3}$$

*Corresponding author. Email: B.N.Ryland@massey.ac.nz

*International Journal of Computer Mathematics*
ISSN: 0020-7160 print/ISSN 1029-0265 online © 200x Taylor & Francis
http://www.tandf.co.uk/journals
DOI: 10.1080/0020716YYxxxxxxxx

holds, where $\omega = \frac{1}{2}\mathbf{K}\mathrm{d}z \wedge \mathrm{d}z$ and $\kappa = \frac{1}{2}\mathbf{L}\mathrm{d}z \wedge \mathrm{d}z$ are 2-forms and $\mathrm{d}z$ satisfies the first variation of the PDE,

$$\mathbf{K}\mathrm{d}z_t + \mathbf{L}\mathrm{d}z_x = D_{zz}S(z)\mathrm{d}z, \tag{4}$$

where $D_{zz}S(z)$ is a symmetric matrix. (The MSCL will depend on the nonlinearity through the linearization along a solution trajectory. That is, (3) holds for the variational equation linearized along a solution, and the solution is nonlinear in general.) By analogy with Hamiltonian ODEs, multisymplectic integrators for multisymplectic PDEs are discretizations for which a discrete analogue of Eq. (3) holds [3], a so-called discrete multisymplectic conservation law (DMSCL). We note immediately that, in contrast to symplecticity (Eq. (1)), an integrator cannot preserve multisymplecticity (Eq. (3)) exactly; different methods preserve different discretizations of Eq. (3). The role of the form of the DMSCL in the behaviour of the method is not yet fully understood.

In particular, for appropriate boundary conditions (e.g. periodic in $x$), Eq. (3) implies that the flow is symplectic:

$$\partial_t \int \omega \, \mathrm{d}x = 0. \tag{5}$$

It is possible to derive integrators which formally possess a DMSCL by replacing the derivatives in Eq. (2) by an approximation of Runge–Kutta (RK) or partitioned Runge–Kutta (PRK) type. The Preissman box scheme (the implicit midpoint rule in space and time) is the most famous such example; it has been applied to many multi-Hamiltonian PDEs. We give an example of such a derivation below for a PRK spatial semi-discretization. However, such a formal derivation omits many key steps which have to be completed in order to define a useful numerical method. The problems that can arise include:

(i) there may be no obvious choice of dependent variables;
(ii) the discrete equations may not be well-defined locally (i.e., there may not be one equation per dependent variable per cell);
(iii) the discrete equations may not be well-defined globally (i.e., there may not be one equation per dependent variable across all spatial grid points when boundary conditions are imposed);
(iv) the discrete equations may not have a solution, or may not have a unique solution or isolated solutions.

These problems are already apparent with the most popular multisymplectic integrator, the box scheme. With periodic boundary conditions in one space dimension, the discrete equations typically only have solutions with an odd number of grid points. With an even number of grid points they have no solution (nonlinear problems) or an infinite number of solutions (linear problems). With higher order RK methods the problems are even worse [4].

The same problems arise in a discrete Lagrangian approach [5]. The variational approach generates discrete equations with a DMSCL, but there is no guarantee that they define a numerical method. Indeed, RK and PRK methods themselves can be derived variationally.

Because there is as yet no general solution to the above problems—for all PDEs of the form of Eq. (2) and for all PRK methods, say—we make in this paper a careful study of various methods applied to one particular equation, the nonlinear Schrödinger (NLS) equation. The previously published multisymplectic integrators for NLS [6–14] are all implicit and based on the box scheme. The cost of this implicit method has been criticised [15], perhaps justifiably, since explicit symplectic integrators for NLS have been known for many decades (based on splitting) [16] and are probably the current method of choice in applications. We therefore want to explore explicit multisymplectic integrators for NLS. This rules out a spatial discretization by RK (such as the box scheme) and we therefore turn to PRK. It is known that these can be explicit—indeed, the explicit 5-point central difference for the wave equation is a PRK discretization in space and time. Even so, for PRK methods the following problems may arise in addition to those above:

(v) the ODEs obtained from a PRK discretization in space may not be explicit;
(vi) if they are explicit, they may not be separable, i.e., they may not allow an explicit PRK discretization in time.

The resolution to (i)-(vi) depends on the PDE, especially on the structure of $\mathbf{K}$, $\mathbf{L}$ and $S(z)$. For the KdV equation, applying the simplest PRK method in space (Lobatto IIIA–IIIB, see below) does *not* give rise to explicit ODEs [17]. On the other hand, if one does get explicit ODEs then this will generally avoid problems (iii) and (iv).

The definition of a PRK method involves a partitioning of the dependent variables $z$ into two sets, with a different set of RK coefficients being applied to each. Previous studies of multisymplectic integrators based on PRK [18] have used the same partitioning of variables for the space and time discretizations and have identified many special cases of $\mathbf{K}$ and $\mathbf{L}$ and choices of PRK method for which the method formally has a DMSCL. However, these cases do not cover the NLS equation. We therefore introduce in this paper a generalization which allows different partitioning of the variables in space and in time, which can be multisymplectic and which does cover the NLS equation.

Implicit PRK methods are not widely used for Hamiltonian ODEs (explicit PRK methods are equivalent to splitting methods), perhaps because of the apparently superior properties of Gaussian RK (GRK) methods. They were originally proposed for use in constrained systems, to which GRK did not appear to apply [19]. An exception is the lowest order Lobatto IIIA–IIIB or "generalized leapfrog" method, which has somewhat simpler implicit equations than the higher order methods. Depending on the structure of the problem, these equations may be able to be solved much more quickly than those of a general implicit method [20].

However, when used as a spatial discretization, the distinction between explicit and implicit disappears, and PRK methods appear to have several advantages over RK methods in multisymplectic integration.

As far as we are aware, there have been no previous studies of the multisymplecticity of splitting methods for time integration. We address this question here by applying them to the time integration of the ODEs arising from a spatial semi-discretization that does have a semi-discrete MSCL. We show that splitting methods can be multisymplectic. However, the resulting DMSCLs can have a different character to those arising from PRK and the question arises as to the significance of the precise form of the DMSCL possessed by a method. We have found no precise or universally-agreed definition of a DMSCL in the literature, so it is not clear, for example, how one could show that a particular method is *not* multisymplectic.

In this paper we are concerned with the focussing cubic nonlinear Schrödinger (NLS) equation [21],

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \tag{6}$$

which can be written in the form of Eq. (2) [22] with $\psi = p + iq$, $z = (p, q, v, w)^T$,

$$\mathbf{K} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \tag{7}$$

and $S(z) = -\frac{1}{2}(p^2 + q^2)^2 - \frac{1}{2}(v^2 + w^2)$, i.e.,

$$\begin{aligned} -q_t + v_x &= -2(q^2 + p^2)p, \\ p_t + w_x &= -2(q^2 + p^2)q, \\ -p_x &= -v, \\ -q_x &= -w. \end{aligned} \tag{8}$$

Eliminating $v$ and $w$ gives

$$\begin{aligned} q_t &= p_{xx} + 2(q^2 + p^2)p, \\ p_t &= -q_{xx} - 2(q^2 + p^2)q. \end{aligned} \tag{9}$$

We will move between the set of four 1st order real PDEs (Eq. (8)) and the two real (or one complex) PDEs (Eq. (9)) as convenient.

The first variation equation is written in the variables $\mathrm{d}z = (\mathrm{d}p, \mathrm{d}q, \mathrm{d}v, \mathrm{d}w)^T$ with the same $\mathbf{K}$ and $\mathbf{L}$ and the symmetric matrix $D_{zz}S(z)$ given by

$$D_{zz}S(z) = \begin{bmatrix} -6p^2 - 2q^2 & -4qp & 0 & 0 \\ -4pq & -2p^2 - 6q^2 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}. \tag{10}$$

Thus, the 2-forms $\omega$ and $\kappa$ which make up the multisymplectic conservation law are given by

$$\begin{aligned} \omega &= \mathrm{d}p \wedge \mathrm{d}q, \\ \kappa &= \mathrm{d}v \wedge \mathrm{d}p + \mathrm{d}w \wedge \mathrm{d}q. \end{aligned} \tag{11}$$

The contents of the remaining sections of this paper are as follows. In Section 2 we discuss the nonlinear Schrödinger equation and the ODEs obtained by applying a semi-discretization in space with Lobatto IIIA–IIIB. In Section 3 we will consider three time integrators applied to these ODEs. In Section 3.1 we will focus on the integrator obtained by applying the second order Lobatto IIIA–IIIB discretization in time to the ODEs obtained in Section 2. We will show that the integrator is explicit and that it satisfies the local discrete multisymplectic conservation law given by Eq. (33). In Section 3.2.1 we will be concerned with the standard (linear–nonlinear) splitting of the ODEs obtained in Section 2. We will show that the splitting also gives rise to an explicit multisymplectic integrator, but neither the integrator nor its corresponding multisymplectic conservation law are local. In Section 3.2.2 we study another (real–imaginary) splitting, that is explicit and does have a local multisymplectic conservation law. In Section 4 we discuss conservation laws for NLS that arise from a multisymplectic form of Noether's theorem. Lastly, in Section 5 we consider the definition of discrete multisymplecticity.

## 2. Spatial semi-discretization

We consider a class of spatial semi-discretizations of the multi-Hamiltonian PDE (2) in which the dependent variables $z \in \mathbb{R}^n$ are partitioned into two sets, $z^{(1)} \in \mathbb{R}^{n_1}$ and $z^{(2)} \in \mathbb{R}^{n_2}$, with $n_1 + n_2 = n$. We introduce a grid in space with grid points (or *nodes*) $x_i$, taken for convenience only to have equal spacing $\Delta x$. The values of the variables $z$ at the nodes are given by $z_j$. An $r$-stage PRK discretization in space applied to this system is a set of equations coupling the $z_j$ to the stage values $Z_i$ at $r$ internal stages given by (at node 0)

$$\begin{aligned} Z_i^{(1)} &= z_0^{(1)} + \Delta x \sum_{j=1}^{r} a_{ij} \partial_x Z_j^{(1)}, \\ z_1^{(1)} &= z_0^{(1)} + \Delta x \sum_{j=1}^{r} b_j \partial_x Z_j^{(1)}, \\ Z_i^{(2)} &= z_0^{(2)} + \Delta x \sum_{j=1}^{r} \hat{a}_{ij} \partial_x Z_j^{(2)}, \\ z_1^{(2)} &= z_0^{(2)} + \Delta x \sum_{j=1}^{r} \hat{b}_j \partial_x Z_j^{(2)}. \end{aligned} \tag{12}$$

where the new variables $\partial_x Z_j^{(i)}$ satisfy the PDE (2), i.e., $\frac{\partial}{\partial t}\mathbf{K}Z_j^{(i)} + \mathbf{L}\partial_x Z_j^{(i)} = \nabla S(Z_j^{(i)})$. In contrast to the use of PRK for time integration (i.e., when the dimension of space-time is 1), in which the dependent variables are $z_i$ and the above equations determine $Z_j$ and define a map from $z_0$ to $z_1$, when used as a spatial semi-discretization (i.e., when the dimension of space-time is greater than 1) the dependent variables will typically be the stage values $Z_j$; the node values $z_i$ and the $\partial_x Z_j^{(i)}$ will be eliminated using the PDE to yield a set of ODEs in time for the $Z_j$. This elimination step depends on the structure ($\mathbf{K}$, $\mathbf{L}$, and $S$) of the PDE. However, it is a remarkable fact that regardless of this structure, Eq. (12) formally possesses a semi-discrete multisymplectic conservation law that approximates the integral of Eq. (3) over the domain $[x_0, x_1]$, i.e.,

$$\int_{x_0}^{x_1} \partial_t \omega(t,x)\,\mathrm{d}x + \kappa(t,x_1) - \kappa(t,x_0) = 0. \tag{13}$$

Theorem 2.1 *Given a multi-Hamiltonian PDE (2) and a PRK discretization (12) in which the coefficients satisfy $b_j = \hat{b}_j$ and*

$$b_i\hat{b}_j - b_i\hat{a}_{ij} - \hat{b}_j a_{ji} = 0 \quad \textit{for all } i,j, \tag{14}$$

*if the variables can be partitioned into distinct sets $z^{(1)}$ and $z^{(2)}$ such that the wedge product $\mathbf{L}\mathrm{d}z \wedge \mathrm{d}z$ only has terms of the form $\mathrm{d}z_i^{(1)} \wedge \mathrm{d}z_j^{(2)}$, then the discretization formally satisfies the semi-discrete multisymplectic conservation law*

$$\Delta x \sum_j b_j \partial_t \omega_j(t) + \kappa_1(t) - \kappa_0(t) = 0. \tag{15}$$

The proof of Theorem 2.1 is given in Appendix A.

The particular class of PRK discretizations that we will be concerned with in this paper are known as Lobatto IIIA–IIIB. For $r$-stage Lobatto IIIA–IIIB, the coefficients $a_{ij}$, $\hat{a}_{ij}$ and $\hat{b}_j = b_j$ are determined by [1]

$$\begin{aligned}
B(r):&\qquad \sum_{i=1}^{r} b_i c_i^{k-1} = \frac{1}{k}, \quad 1 \le k \le r,\\
C(r):&\qquad \sum_{j=1}^{r} a_{ij} c_j^{k-1} = \frac{1}{k}c_i^k, \quad 1 \le i \le r,\ 1 \le k \le, r\\
D(r):&\qquad \sum_{i=1}^{r} b_i c_i^{k-1}\hat{a}_{ij} = \frac{1}{k} b_j(1-c_j^k), \quad 1 \le j \le r,\ 1 \le k \le r
\end{aligned} \tag{16}$$

and the $c_i$ are zeros of the Lobatto quadrature polynomial

$$\frac{\mathrm{d}^{r-2}}{\mathrm{d}x^{r-2}}\left(x^{r-1}(x-1)^{r-1}\right). \tag{17}$$

Discretizing the NLS equation in space by applying Lobatto IIIA to the variables $p$ and $q$ and Lobatto

IIIB to the variables $v$ and $w$ results in the following set of equations

$$\begin{aligned} P_i &= p_0 + \Delta x \sum_j a_{ij} V_j, \\ Q_i &= q_0 + \Delta x \sum_j a_{ij} W_j, \\ V_i &= v_0 + \Delta x \sum_j \hat{a}_{ij} (\partial_t Q_j - 2(P_j^2 + Q_j^2) P_j), \\ W_i &= w_0 + \Delta x \sum_j \hat{a}_{ij} (-\partial_t P_j - 2(P_j^2 + Q_j^2) Q_j), \\ p_1 &= p_0 + \Delta x \sum_j b_j V_j, \\ q_1 &= q_0 + \Delta x \sum_j b_j W_j, \\ v_1 &= v_0 + \Delta x \sum_j \hat{b}_j (\partial_t Q_j - 2(P_j^2 + Q_j^2) P_j), \\ w_1 &= w_0 + \Delta x \sum_j \hat{b}_j (-\partial_t P_j - 2(P_j^2 + Q_j^2) Q_j). \end{aligned} \tag{18}$$

This partitioning of the variables satisfies the conditions of Theorem 2.1, thus the discretization satisfies a semi-discrete multisymplectic conservation law of the form of Eq. (15).

In a forthcoming paper [23] we give sufficient conditions on $\mathbf{K}$, $\mathbf{L}$, and $S(z)$ for Lobatto IIIA–IIIB to generate an explicit set of ODEs for any $r$ and an algorithm for generating them. The NLS equation does satisfy these conditions. Here, we confine ourselves to illustrating the result for NLS for $r = 2$, 3, and 4.

First, let $r = 2$. Eliminating the variables $v_i$, $V_j$, $w_i$ and $W_j$ from Eq. (18) and noting that $P_1 = p_0$, $P_2 = p_1$, $Q_1 = q_0$ and $Q_2 = q_1$, this system is reduced to two coupled ODEs at each gridpoint in the variables $p_i$ and $q_i$, namely

$$\begin{aligned} \partial_t p_i &= -\frac{1}{\Delta x^2}(q_{i-1} - 2q_i + q_{i+1}) - 2(p_i^2 + q_i^2) q_i, \\ \partial_t q_i &= \frac{1}{\Delta x^2}(p_{i-1} - 2p_i + p_{i+1}) + 2(p_i^2 + q_i^2) p_i. \end{aligned} \tag{19}$$

Note that this amounts to replacing the $v_x$ and $w_x$ terms in Eq. (9) by the central differences of $p_{xx}$ and $q_{xx}$ respectively.

While Eq. (18) satisfies a multisymplectic conservation law of the form of Eq. (15), Eq. (19) is written with only a subset of the variables so it is desirable to have the semi-discrete multisymplectic conservation law written in terms of these variables.

Theorem 2.2 *The ODEs (19) satisfy the discrete multisymplectic conservation law*

$$\partial_t (\mathrm{d}p_i \wedge \mathrm{d}q_i) + \frac{1}{\Delta x^2}\Big((\mathrm{d}p_{i+1} + \mathrm{d}p_{i-1}) \wedge \mathrm{d}p_i + (\mathrm{d}q_{i+1} + \mathrm{d}q_{i-1}) \wedge \mathrm{d}q_i\Big) = 0. \tag{20}$$

*Proof* Although Eq. (20) can be directly verified from Eq. (19), we show here that it follows as a result of Eq. (18) satisfying the DMSCL (15).

Beginning with $\omega_j = \mathrm{d}P_j \wedge \mathrm{d}Q_j$ we can write the first term in Eq. (15) as

$$\begin{aligned}\Delta x \sum_j b_j \partial_t \omega_j &= \frac{\Delta x}{2} \sum_j \partial_t(\mathrm{d}P_j \wedge \mathrm{d}Q_j) \\ &= \frac{\Delta x}{2} \left(\partial_t(\mathrm{d}P_1 \wedge \mathrm{d}Q_1) + \partial_t(\mathrm{d}P_2 \wedge \mathrm{d}Q_2)\right) \\ &= \frac{\Delta x}{2} \left(\partial_t(\mathrm{d}p_i \wedge \mathrm{d}q_i) + \partial_t(\mathrm{d}p_{i+1} \wedge \mathrm{d}q_{i+1})\right)\end{aligned}$$

Noting that $\kappa_i = \mathrm{d}v_i \wedge \mathrm{d}p_i + \mathrm{d}w_i \wedge \mathrm{d}q_i$, we can write Eq. (15) as

$$\frac{1}{2} \left(\partial_t(\mathrm{d}p_i \wedge \mathrm{d}q_i) + \partial_t(\mathrm{d}p_{i+1} \wedge \mathrm{d}q_{i+1})\right) + \frac{1}{\Delta x} \left(\mathrm{d}v_{i+1} \wedge \mathrm{d}p_{i+1} + \mathrm{d}w_{i+1} \wedge \mathrm{d}q_{i+1} - \mathrm{d}v_i \wedge \mathrm{d}p_i - \mathrm{d}w_i \wedge \mathrm{d}q_i\right) = 0 \tag{21}$$

Now,

$$\mathrm{d}V_1 = \mathrm{d}V_2 = \mathrm{d}v_i + \frac{\Delta x}{2}(\partial_t \mathrm{d}Q_1 - (6(P_1)^2 + 2(Q_1)^2)\mathrm{d}P_1 - 4P_1Q_1\mathrm{d}Q_1) \tag{22}$$

and

$$\mathrm{d}p_{i+1} = \mathrm{d}p_i + \frac{\Delta x}{2}(\mathrm{d}V_1 + \mathrm{d}V_2) \tag{23}$$

so

$$\begin{aligned}\mathrm{d}v_{i+1} &= \mathrm{d}v_i + \frac{\Delta x}{2} \sum_j (\partial_t \mathrm{d}Q_j - (6(P_j)^2 + 2(Q_j)^2)\mathrm{d}P_j - 4P_jQ_j\mathrm{d}Q_j) \\ &= \mathrm{d}V_1 + \frac{\Delta x}{2}(\partial_t \mathrm{d}q_{i+1} - (6(p_{i+1})^2 + 2(q_{i+1})^2)\mathrm{d}p_{i+1} - 4p_{i+1}q_{i+1}\mathrm{d}q_{i+1}), \\ &= \frac{1}{\Delta x}(\mathrm{d}p_{i+1} - \mathrm{d}p_i) + \frac{\Delta x}{2}(\partial_t \mathrm{d}q_{i+1} - (6(p_{i+1})^2 + 2(q_{i+1})^2)\mathrm{d}p_{i+1} - 4p_{i+1}q_{i+1}\mathrm{d}q_{i+1}),\end{aligned} \tag{24}$$

and similarly for $\mathrm{d}w_{i+1}$. Substituting for $\mathrm{d}v_{i+1}$, $\mathrm{d}v_i$, $\mathrm{d}w_{i+1}$ and $\mathrm{d}w_i$ in Eq. (21) gives

$$\begin{aligned}&\frac{1}{2}(\partial_t(\mathrm{d}p_i \wedge \mathrm{d}q_i) + \partial_t(\mathrm{d}p_{i+1} \wedge \mathrm{d}q_{i+1})) \\ &\quad + \frac{1}{\Delta x}\Big( (\frac{1}{\Delta x}(\mathrm{d}p_{i+1} - \mathrm{d}p_i) + \frac{\Delta x}{2}(\partial_t \mathrm{d}q_{i+1} - (6(p_{i+1})^2 + 2(q_{i+1})^2)\mathrm{d}p_{i+1} - 4p_{i+1}q_{i+1}\mathrm{d}q_{i+1})) \wedge \mathrm{d}p_{i+1} \\ &\quad + (\frac{1}{\Delta x}(\mathrm{d}q_{i+1} - \mathrm{d}q_i) + \frac{\Delta x}{2}(-\partial_t \mathrm{d}p_{i+1} - 4p_{i+1}q_{i+1}\mathrm{d}p_{i+1} - (2(p_{i+1})^2 + 6(q_{i+1})^2)\mathrm{d}q_{i+1})) \wedge \mathrm{d}q_{i+1} \\ &\quad - (\frac{1}{\Delta x}(\mathrm{d}p_i - \mathrm{d}p_{i-1}) + \frac{\Delta x}{2}(\partial_t \mathrm{d}q_i - (6(p_i)^2 + 2(q_i)^2)\mathrm{d}p_i - 4p_iq_i\mathrm{d}q_i)) \wedge \mathrm{d}p_i \\ &\quad - (\frac{1}{\Delta x}(\mathrm{d}q_i - \mathrm{d}q_{i-1}) + \frac{\Delta x}{2}(-\partial_t \mathrm{d}p_i - 4p_iq_i\mathrm{d}p_i - (2(p_i)^2 + 6(q_i)^2)\mathrm{d}q_i)) \wedge \mathrm{d}q_i \Big) = 0.\end{aligned} \tag{25}$$

Since $\mathrm{d}p_i \wedge \mathrm{d}p_i = 0$ and $\mathrm{d}q_i \wedge \mathrm{d}p_i = -\mathrm{d}p_i \wedge \mathrm{d}q_i$, this simplifies to

$$\begin{aligned}\frac{1}{2}(\partial_t(\mathrm{d}p_i \wedge \mathrm{d}q_i) + \partial_t(\mathrm{d}p_{i+1} \wedge \mathrm{d}q_{i+1}))\\ + \frac{1}{\Delta x^2}\left(\mathrm{d}p_{i+1} \wedge \mathrm{d}p_i + \mathrm{d}q_{i+1} \wedge \mathrm{d}q_i - \mathrm{d}p_i \wedge \mathrm{d}p_{i-1} - \mathrm{d}q_i \wedge \mathrm{d}q_{i-1}\right)\\ + \frac{1}{2}\left(-\mathrm{d}p_{i+1} \wedge \partial_t \mathrm{d}q_{i+1} - \partial_t \mathrm{d}p_{i+1} \wedge \mathrm{d}q_{i+1} + \mathrm{d}p_i \wedge \partial_t \mathrm{d}q_i + \partial_t \mathrm{d}p_i \wedge \mathrm{d}q_i\right) = 0,\end{aligned} \tag{26}$$

which further simplifies to Eq. (20). □

Eq. (19) can be written in terms of the original variable $\psi = p + iq$ as

$$i\partial_t \psi_i = -\frac{1}{\Delta x^2}(\psi_{i-1} - 2\psi_i + \psi_{i+1}) - 2|\psi|^2\psi. \tag{27}$$

with semi-discrete MSCL

$$i\partial_t(\mathrm{d}\psi_i \wedge \mathrm{d}\bar{\psi}_i) + \frac{1}{\Delta x^2}\left(\mathrm{d}\psi_{i+1} \wedge \mathrm{d}\bar{\psi}_i + \mathrm{d}\bar{\psi}_{i+1} \wedge \mathrm{d}\psi_i - \mathrm{d}\psi_i \wedge \mathrm{d}\bar{\psi}_{i-1} - \mathrm{d}\bar{\psi}_i \wedge \mathrm{d}\psi_{i-1}\right) = 0. \tag{28}$$

Local, explicit, multisymplectic methods for any $r$ can be obtained in this way; we give the $r = 3$ and $r = 4$ cases below. They do not have an interpretation as classical finite differences. Note that the ODEs for the first and last stages (which coincide with the node values) couple the stage variables of 3 adjacent cells, while the ODEs for the internal stages only couple the stage variables within a cell.

For $r = 3$ the ODEs are

$$\begin{aligned}\partial_t P_{i,1} &= -\frac{1}{\Delta x^2}(-Q_{i-1,1} + 8Q_{i-1,2} - 14Q_{i,1} + 8Q_{i,2} - Q_{i+1,1}) - 2(P_{i,1}^2 + Q_{i,1}^2)Q_{i,1},\\ \partial_t P_{i,2} &= -\frac{1}{\Delta x^2}(4Q_{i,1} - 8Q_{i,2} + 4Q_{i+1,1}) - 2(P_{i,2}^2 + Q_{i,2}^2)Q_{i,2},\\ \partial_t P_{i,3} &= \partial_t P_{i+1,1},\\ \partial_t Q_{i,1} &= \frac{1}{\Delta x^2}(-P_{i-1,1} + 8P_{i-1,2} - 14P_{i,1} + 8P_{i,2} - P_{i+1,1}) + 2(P_{i,1}^2 + Q_{i,1}^2)P_{i,1},\\ \partial_t Q_{i,2} &= \frac{1}{\Delta x^2}(4P_{i,1} - 8P_{i,2} + 4P_{i+1,1}) + 2(P_{i,2}^2 + Q_{i,2}^2)P_{i,2},\\ \partial_t Q_{i,3} &= \partial_t Q_{i+1,1},\end{aligned} \tag{29}$$

where $P_{i,j}$ is the $j$th internal stage for cell $i$, $P_{i,1} = p_i$ and $Q_{i,1} = q_i$ .

For $r = 4$ the ODEs are

$$
\begin{aligned}
\partial_t P_{i,1} &= -\frac{1}{\Delta x^2}(Q_{i-1,1} + \frac{1}{2}(25 - 15\sqrt{5})Q_{i-1,2} + \frac{1}{2}(25 + 15\sqrt{5})Q_{i-1,3} - 52Q_{i,1} \\
&\quad + \frac{1}{2}(25 + 15\sqrt{5})Q_{i,2} + \frac{1}{2}(25 - 15\sqrt{5})Q_{i,3} + Q_{i+1,1}) - 2(P_{i,1}^2 + Q_{i,1}^2)Q_{i,1}, \\
\partial_t P_{i,2} &= -\frac{1}{\Delta x^2}((5 + 3\sqrt{5})Q_{i,1} - 20Q_{i,2} + 10Q_{i,3} + (5 - 3\sqrt{5})Q_{i+1,1}) - 2(P_{i,2}^2 + Q_{i,2}^2)Q_{i,2}, \\
\partial_t P_{i,3} &= -\frac{1}{\Delta x^2}((5 - 3\sqrt{5})Q_{i,1} + 10Q_{i,2} - 20Q_{i,3} + (5 + 3\sqrt{5})Q_{i+1,1}) - 2(P_{i,3}^2 + Q_{i,3}^2)Q_{i,3}, \\
\partial_t P_{i,4} &= \partial_t P_{i+1,1}, \\
\partial_t Q_{i,1} &= \frac{1}{\Delta x^2}(P_{i-1,1} + \frac{1}{2}(25 - 15\sqrt{5})P_{i-1,2} + \frac{1}{2}(25 + 15\sqrt{5})P_{i-1,3} - 52P_{i,1} \\
&\quad + \frac{1}{2}(25 + 15\sqrt{5})P_{i,2} + \frac{1}{2}(25 - 15\sqrt{5})P_{i,3} + P_{i+1,1}) - 2(P_{i,1}^2 + Q_{i,1}^2)P_{i,1}, \\
\partial_t Q_{i,2} &= \frac{1}{\Delta x^2}((5 + 3\sqrt{5})P_{i,1} - 20P_{i,2} + 10P_{i,3} + (5 - 3\sqrt{5})P_{i+1,1}) - 2(P_{i,2}^2 + Q_{i,2}^2)P_{i,2}, \\
\partial_t Q_{i,3} &= \frac{1}{\Delta x^2}((5 - 3\sqrt{5})P_{i,1} + 10P_{i,2} - 20P_{i,3} + (5 + 3\sqrt{5})P_{i+1,1}) - 2(P_{i,3}^2 + Q_{i,3}^2)P_{i,3}, \\
\partial_t Q_{i,4} &= \partial_t Q_{i+1,1},
\end{aligned} \tag{30}
$$

where $P_{i,1} = p_i$ and $Q_{i,1} = q_i$.

The semi-discrete multisymplectic conservation laws for $r = 3$ and $r = 4$ Lobatto IIIA–IIIB can be obtained by plugging the variational equivalents of Eqs. (29) and (30) respectively into Eq. (15); however, they do not reduce to an equation as elegant as Eq. (20).

For many schemes (e.g. implicit midpoint, higher order GRK), when boundary conditions are imposed the methods either do not remain well-defined or they require extra conditions to be so [4,17]. In contrast, the Lobatto IIIA–IIIB methods given above remain well-defined under periodic, Dirichlet or Neumann boundary conditions without any further restrictions. For example, $r = 3$ Lobatto IIIA–IIIB with Neumann boundary conditions, $\psi_x = 0$ (i.e. $v = 0$, $w = 0$), applied to the left boundary as $v_1 = w_1 = 0$ leads to the following ODEs:

$$
\begin{aligned}
\partial_t P_{1,1} &= -\frac{1}{\Delta x^2}(-14Q_{1,1} + 16Q_{1,2} - 2Q_{2,1}) - 2(P_{1,1}^2 + Q_{1,1}^2)Q_{1,1}, \\
\partial_t Q_{1,1} &= \frac{1}{\Delta x^2}(-14P_{1,1} + 16P_{1,2} - 2P_{2,1}) + 2(P_{1,1}^2 + Q_{1,1}^2)P_{1,1}.
\end{aligned} \tag{31}
$$

These ODEs are equivalent to the first and fourth line of Eq. (29) where the points outside the domain are treated as phantom points, i.e. $Q_{0,1} = Q_{2,1}$ and $Q_{0,2} = Q_{1,2}$.

It is a great advantage to have local ODEs as then the well-posedness of various boundary conditions can be determined purely locally.

Note that Lobatto IIIA–IIIB also gives an explicit multisymplectic semi-discretization on non-constant-spaced grids.

## 3. Time integration

We will consider the time integration of the ODEs (19) by 3 different methods: one PRK method (second-order Lobatto IIIA–IIIB) and two splitting methods, the classical linear–nonlinear splitting and a real–imaginary–nonlinear splitting.

### 3.1. *Integration by Lobatto IIIA–IIIB discretization*

Previous studies of multisymplectic PRK methods [18] have established that a full discretization of a multi-Hamiltonian PDE satisfying certain conditions on $\mathbf{K}$ and $\mathbf{L}$ will formally possess a DMSCL. In particular, these conditions require the choice of the same partitioning of variables in space and time. When applied to NLS, the partitioning used so far, namely $z^{(1)} = (p, q)$, $z^{(2)} = (u, v)$ leads to a set of ODEs for $z^{(1)}$ alone. Therefore, any PRK applied to these ODEs with this partitioning will reduce to an RK method in $z^{(1)}$, such as the midpoint rule. Since we are looking for explicit integrators we need to relax this assumption.

In [23] it is shown that a symplectic PRK time integrator with *any* partitioning of the variables, applied to the semi-discrete PRK system, is multisymplectic. Standard symplectic PRK methods are defined for ODEs with canonical symplectic structure; this is extended to noncanonical structure by requiring that the coefficients satisfy $b_j = \hat{b}_j$ and

$$b_i\hat{b}_j - b_i\hat{a}_{ij} - \hat{b}_j a_{ji} = 0 \quad \text{for all } i, j, \tag{32}$$

and the variables can be separated into distinct sets $z^{(3)} \in \mathbb{R}^{n_3}$ and $z^{(4)} \in \mathbb{R}^{n_4}$ $(n = n_3 + n_4)$ such that the wedge product $\mathbf{K}\mathrm{d}z \wedge \mathrm{d}z$ only has terms of the form $\mathrm{d}z_i^{(3)} \wedge \mathrm{d}z_j^{(4)}$. Then the equations one obtains formally satisfy the fully discrete multisymplectic conservation law

$$\Delta x \sum_j b_j(\omega_j^1 - \omega_j^0) + \Delta t \sum_m B_m(\kappa_1^m - \kappa_0^m) = 0, \tag{33}$$

where $\omega_j^1 = \omega(t_1, x_0 + c_j\Delta x)$, $\omega_j^0 = \omega(t_0, x_0 + c_j\Delta x)$, $\kappa_1^m = \kappa(t_0 + C_m\Delta t, x_1)$, $\kappa_0^m = \kappa(t_0 + C_m\Delta t, x_0)$, $b_j$ and $c_j$ are the coefficients in the spatial PRK discretization and $B_m$ and $C_m$ are the coefficients in the temporal PRK discretization. Eq. (33) is an approximation to the integral

$$\int_0^{\Delta x} (\omega(x, \Delta t) - \omega(x, 0))\,\mathrm{d}x + \int_0^{\Delta t} (\kappa(\Delta x, t) - \kappa(0, t))\,\mathrm{d}t = 0, \tag{34}$$

We now choose the partitioning $z^{(3)} = (p, v)$, $z^{(4)} = (q, w)$. The variables $v$ and $w$ have been eliminated in (19), so we are left with a standard $p$–$q$ partitioning. Second order Lobatto IIIA–IIIB with this partitioning is commonly known as generalized leapfrog which, for an ODE $q_t = f(q, p)$, $p_t = g(q, p)$, takes the form [20]

$$\begin{aligned}
q^{n+\frac{1}{2}} &= q^n + \frac{\Delta t}{2} f(q^{n+\frac{1}{2}}, p^n),\\
p^{n+1} &= p^n - \frac{\Delta t}{2}\left(g(q^{n+\frac{1}{2}}, p^n) + g(q^{n+\frac{1}{2}}, p^{n+1})\right),\\
q^{n+1} &= q^{n+\frac{1}{2}} + \frac{\Delta t}{2} f(q^{n+\frac{1}{2}}, p^{n+1}).
\end{aligned} \tag{35}$$

In general it is an implicit method. Applied to (19), we obtain the integrator that maps $(p_i^n, q_i^n)$ to $(p_i^{n+1}, q_i^{n+1})$ in the following way:

$$\begin{aligned}
q_i^{n+\frac{1}{2}} &= q_i^n + \frac{\Delta t}{2}\frac{1}{\Delta x^2}(p_{i-1}^n - 2p_i^n + p_{i+1}^n) + \Delta t((q_i^{n+\frac{1}{2}})^2 + (p_i^n)^2)p_i^n,\\
p_i^{n+1} &= p_i^n - \Delta t(q_{i-1}^{n+\frac{1}{2}} - 2q_i^{n+\frac{1}{2}} + q_{i+1}^{n+\frac{1}{2}}) - \Delta t((p_i^n)^2 + (p_i^{n+1})^2 + 2(q_i^{n+\frac{1}{2}})^2)q_i^{n+\frac{1}{2}},\\
q_i^{n+1} &= q_i^{n+\frac{1}{2}} + \frac{\Delta t}{2}\frac{1}{\Delta x^2}(p_{i-1}^{n+1} - 2p_i^{n+1} + p_{i+1}^{n+1}) + \Delta t((q_i^{n+\frac{1}{2}})^2 + (p_i^{n+1})^2)p_i^{n+1}.
\end{aligned} \tag{36}$$

We observe that the only nonlinearities enter as scalar quadratic equations which can be solved explicitly. Furthermore, one of the solutions to the quadratic is $\mathcal{O}(1)$ while the other is $\mathcal{O}(\Delta t^{-1})$, so the first solution is always taken.

It can be noted from Eqs. (29) and (30) that varying $r$ only modifies the linear terms of the ODEs, i.e., only modifies the approximation of the spatial derivatives. This is shown in general for an $r$-stage Lobatto IIIA–IIIB discretization in [23]. Thus, with the above partitioning of the variables, an $r$-stage in space and second order in time explicit multisymplectic integrator for NLS can be constructed by applying an $r$-stage Lobatto IIIA–IIIB discretization in space and generalized leap-frog in time.

However, applying a higher order Lobatto IIIA–IIIB discretization in time to Eq. (19) with this partitioning of the variables couples together the nonlinear terms and the resulting method is fully implicit. Instead, a higher order, explicit integrator can be obtained by composition.

THEOREM 3.1 *For second order Lobatto IIIA–IIIB with partitioning $\{(p,q),(v,w)\}$ in space and $\{(p,v),(q,w)\}$ in time applied to the cubic NLS equation ($\psi_t+\psi_{xx}+2|\psi|^2=0$) the discrete multisymplectic conservation law given in Eq. (33) can be written in terms of the local values of $p$ and $q$ as*

$$\begin{aligned}\Big(\frac{1}{\Delta t}+2p_i^{n+1}q_i^{n+\frac12}\Big)\mathrm{d}p_i^{n+1}\wedge \mathrm{d}q_i^{n+\frac12}-\Big(\frac{1}{\Delta t}+2p_i^{n}q_i^{n-\frac12}\Big)\mathrm{d}p_i^{n}\wedge \mathrm{d}q_i^{n-\frac12}&\\ +\frac{1}{\Delta x^2}\Big((\mathrm{d}p_{i+1}^n+\mathrm{d}p_{i-1}^n)\wedge \mathrm{d}p_i^n+(\mathrm{d}q_{i+1}^{n+\frac12}+\mathrm{d}q_{i-1}^{n+\frac12})\wedge \mathrm{d}q_i^{n+\frac12}\Big)=0.&\end{aligned}\tag{37}$$

The proof is in Appendix B.

Because of the choice of partitioning, the results of [18] do not establish that (33) in fact holds. Instead, we shall show directly that its consequence, Eq. (37), holds.

THEOREM 3.2 *Second order Lobatto IIIA–IIIB with partitioning $\{(p,q),(v,w)\}$ in space and $\{(p,v),(q,w)\}$ in time applied to the cubic NLS equation ($\psi_t+\psi_{xx}+2|\psi|^2=0$) is multisymplectic with conservation law Eq. (37).*

*Proof* From the second line of Eq. (36) we have

$$\begin{aligned}\mathrm{d}p_i^{n+1}=\Big(1+2\Delta t p_i^{n+1}q_i^{n+\frac12}\Big)^{-1}\Bigg(&\Big(1-2\Delta t p_i^{n}q_i^{n+\frac12}\Big)\mathrm{d}p_i^n\\ &-\frac{\Delta t}{\Delta x^2}\Big(\mathrm{d}q_{i-1}^{n+\frac12}-2\mathrm{d}q_i^{n+\frac12}+\mathrm{d}q_{i+1}^{n+\frac12}\Big)-\Delta t\Big((p_i^n)^2+(p_i^{n+1})^2+(q_i^{n+\frac12})^2\Big)\mathrm{d}q_i^{n+\frac12}\Bigg).\end{aligned}\tag{38}$$

Substituting Eq. (38) into the first term of Eq. (37) gives

$$\Big(\frac{1}{\Delta t}+2p_i^{n+1}q_i^{n+\frac12}\Big)\mathrm{d}p_i^{n+1}\wedge\mathrm{d}q_i^{n+\frac12}=\frac{1}{\Delta t}\Big(1-2\Delta t p_i^nq_i^{n+\frac12}\Big)\mathrm{d}p_i^n\wedge\mathrm{d}q_i^{n+\frac12}-\frac{1}{\Delta x^2}\Big(\mathrm{d}q_{i-1}^{n+\frac12}+\mathrm{d}q_{i+1}^{n+\frac12}\Big)\wedge\mathrm{d}q_i^{n+\frac12}.\tag{39}$$

Combining the first and last lines of Eq. (36) we have

$$\begin{aligned}\mathrm{d}q_i^{n+\frac12}=\Big(1-2\Delta t p_i^{n}q_i^{n+\frac12}\Big)^{-1}\Bigg(&\Big(1+2\Delta t p_i^{n}q_i^{n-\frac12}\Big)\mathrm{d}q_i^{n-\frac12}\\ &+\frac{\Delta t}{\Delta x^2}\Big(\mathrm{d}p_{i-1}^n-2\mathrm{d}p_i^n+\mathrm{d}p_{i+1}^n\Big)+\Delta t\Big(6(p_i^n)^2+(q_i^{n-\frac12})^2+(q_i^{n+\frac12})^2\Big)\mathrm{d}p_i^n\Bigg),\end{aligned}\tag{40}$$

which when substituted into the first $\mathrm{d}q_i^{n+\frac{1}{2}}$ in Eq. (39) gives

$$\left(\frac{1}{\Delta t} + 2p_i^{n+1}q_i^{n+\frac{1}{2}}\right)\mathrm{d}p_i^{n+1}\wedge\mathrm{d}q_i^{n+\frac{1}{2}} = \frac{1}{\Delta t}\left(1 + 2\Delta t p_i^n q_i^{n-\frac{1}{2}}\right)\mathrm{d}p_i^n\wedge\mathrm{d}q_i^{n-\frac{1}{2}} - \frac{1}{\Delta x^2}\left(\mathrm{d}p_{i-1}^n + \mathrm{d}p_{i+1}^n\right)\wedge\mathrm{d}p_i^n - \frac{1}{\Delta x^2}\left(\mathrm{d}q_{i-1}^{n+\frac{1}{2}} + \mathrm{d}q_{i+1}^{n+\frac{1}{2}}\right)\wedge\mathrm{d}q_i^{n+\frac{1}{2}}. \tag{41}$$

Thus the discrete multisymplectic conservation law given by Eq. (37) is satisfied. □

### 3.2. *Integration by symplectic splitting*

For Hamiltonian ODEs, a highly fruitful method for constructing symplectic integrators is based on Hamiltonian vector field splitting [24]. For example, suppose an abstract Hamiltonian system $z_t = \mathbf{J}\nabla_z H(z)$ can be written in the form

$$z_t = \mathbf{J}\nabla_z(H^{(1)}(z) + \cdots + H^{(N)}(z)), \tag{42}$$

where each of the subsystems $z_t = \mathbf{J}\nabla_z H^{(j)}(z)$, $j = 1, \ldots, N$ can be solved exactly. Denote the time-$\Delta t$ solution operator of the $j$th subsystem by $\Psi^{(j)}(\Delta t)$, i.e., $z(\Delta t) = \Psi^{(j)}(\Delta t)z(0)$ satisfies the $j$th flow. Then, since the flow of each subsystem is a symplectic map, and the composition of symplectic maps is again symplectic, the composite map

$$\bar{\Psi}(\Delta t) := \Psi^{(N)}(\Delta t)\circ\cdots\circ\Psi^{(1)}(\Delta t) \tag{43}$$

is symplectic. Furthermore, by the BCH theorem, it is a first order approximation of the exact flow map. Therefore $\bar{\Psi}(\Delta t)$ is a first order symplectic integrator. By varying the lengths of solution intervals of the subsystems, and introducing more elaborate compositions, one can obtain symmetric, symplectic maps of arbitrary accuracy. The exact flow of each subsystem does not have to be available, any consistent symplectic integrator will do. Symplectic splitting methods are the most effective way of obtaining fast, efficient, explicit symplectic methods. For Poisson systems, they are often the only hope of constructing Poisson integrators. For a thorough account see the review article by McLachlan and Quispel [24].

As of yet, splitting methods have not been applied to multisymplectic discretizations of PDEs. Splitting methods are by their nature global constructions, since the PDE along with its boundary conditions are treated as an infinite dimensional ODE. In contrast the multisymplectic theory is local and independent of boundary conditions.

Note that the question of multisymplecticity of splitting methods may be important for multisymplectic systems with nonlinear operators $\mathbf{K}(z)$, $\mathbf{L}(z)$, since Runge–Kutta methods do not preserve such structures. This was briefly noted in [25].

Let us consider a splitting $\mathbf{L} = \sum_{j=1}^N \mathbf{L}^{(j)}$ and $S(z) = \sum_{j=1}^N S^{(j)}(z)$, where each pair forms a multi-Hamiltonian PDE

$$\mathbf{K}z_t + \mathbf{L}^{(j)}z_x = \nabla_z S^{(j)}(z). \tag{44}$$

The flow of each subsystem satisfies a different MSCL

$$\omega_t + \kappa_x^{(j)} = 0, \tag{45}$$

where $\kappa^{(j)} = \frac{1}{2}\mathbf{L}^{(j)}\mathrm{d}z\wedge\mathrm{d}z$. Since the density $\omega$ in each conservation law is the same, the total symplecticity is conserved by each flow, which is the defining property of a symplectic splitting.

Suppose we can solve the subsystems over an interval $\Delta t$. This results in

$$\omega^{(j+1)} - \omega^{(j)} = -\int_0^{\Delta t} \kappa_x^{(j)}(z^{(j)}(x,t))\,\mathrm{d}t, \tag{46}$$

for each subsystem. Combining the subsystems together gives

$$\omega^1 - \omega^0 = \omega^{(N)} - \omega^{(0)} = -\int_0^{\Delta t} \sum_{j=1}^{N} \kappa_x^{(j)}(z^{(j)}(x,t))\,\mathrm{d}t, \tag{47}$$

which is of the same form as (3) but with the 2-forms in the integrals evaluated along different trajectories in phase space.

If $\mathbf{K}$ is degenerate, the projection of $\mathbf{L}z_x = \nabla_z S(z)$ upon the null space of $\mathbf{K}$ will amount to constraints when the PDE is viewed as an infinite dimensional ODE. Often these constraints are removable by substitution. Nonetheless, it would appear necessary to preserve the constraints for each split subsystem. Furthermore, the part of $S(z)$ which defines the constraint should not be split apart from $\mathbf{L}z_x$, since that can lead to strange relations like $z_{j,x} = 0$ for some components $j$, that do not in general satisfy the initial conditions. It is necessary to check that the PDEs (44) are self-consistent for any proposed splitting.

A more concrete example for the NLS equation is given in the next two sections.

**3.2.1. 2 term (linear–nonlinear) splitting.** The standard splitting of the cubic NLS equation is to separate the linear and nonlinear parts [16]. For the first part we take $\mathbf{L}^{(1)} = \mathbf{L}$, $S^{(1)}(z) = -\frac{1}{2}(v^2 + w^2)$, giving the linear PDE $i\psi_t + \psi_{xx} = 0$; for the second part we take $\mathbf{L}^{(2)} = \mathbf{0}$, $S^{(2)} = -\frac{1}{2}(p^2 + q^2)^2$, giving the nonlinear PDE $i\psi_t + 2|\psi|^2\psi = 0$. Note that $v$ and $w$ drop out of this equation entirely and are undetermined; it is possible for the split subsystems to be singular in this way without destroying the method, as long as they are self-consistent.

After discretizing in space, $\psi_{xx}$ becomes $L\psi$ for some operator $L$. (In the original Fourier split-step method, $L$ is the discrete Fourier derivative.) The time-$\Delta t$ map of the first component is $\psi \mapsto \exp(i\Delta t L)\psi$ while the time-$\Delta t$ map of the second component is $\psi \mapsto \exp(i\Delta t|\psi|^2)\psi$.

If the discretizion in space is second order Lobatto IIIA–IIIB, the first part is

$$\begin{aligned} \partial_t p_i &= -\frac{1}{\Delta x^2}(q_{i-1} - 2q_i + q_{i+1}), \\ \partial_t q_i &= \frac{1}{\Delta x^2}(p_{i-1} - 2p_i + p_{i+1}). \end{aligned} \tag{48}$$

These ODEs are multisymplectic with conservation law Eq. (20); the only difference from Eq. (19) is that the nonlinear term, which only appears in $S(z)$, has been dropped. Its flow therefore satisfies Eq. (20) as well, although the differential forms are evaluated on solutions of Eq. (48) instead of (19). One can derive a DMSCL as well, although there seems to be no unique or natural way to do this. For example, integrating Eq. (20) over one time step gives

$$\omega_i^1 - \omega_i^0 + \int_{t_0}^{t_0+\Delta t} \kappa_{i+1}(t) - \kappa_i(t)\,\mathrm{d}t = 0, \tag{49}$$

where $\omega_i = \mathrm{d}p_i \wedge \mathrm{d}q_i$ and $\kappa_i = \frac{1}{\Delta x^2}(\mathrm{d}p_i \wedge \mathrm{d}p_{i-1} + \mathrm{d}q_i \wedge \mathrm{d}q_{i-1})$. The explicit solution in terms of the initial conditions $z^0$ can now be substituted into $\kappa_i(t)$ to give a fully discrete MSCL. However, one could equally well express the solution in terms of the final state $z^1$, or some combination of $z^0$ and $z^1$, giving different DMSCLs. However, although (49) is local in space, the solution to Eq. (48) is not local in space, and therefore the resulting DMSCLs cannot be expected to be local, even though they are the exact solution of the local ODEs (20).

(Note that for the PDE $i\psi_t + \psi_{xx} = 0$, the solution of the local MSCL *is* local in space, by an argument from the method of characteristics; but after spatial discretization the solution of the local MSCL is not local in space.)

The ODEs for the second step are

$$\begin{aligned} \partial_t p_i &= -2(p_i^2 + q_i^2)q_i, \\ \partial_t q_i &= 2(p_i^2 + q_i^2)p_i. \end{aligned} \tag{50}$$

These are Hamiltonian ODEs that satisfy $(\omega_i)_t = 0$, and their solution satisfies $\omega_i^1 = \omega_i^0$. The composition of the two steps therefore satisfies a nonlocal DMSCL. This conservation law is not the same as the original MSCL (20), because during the second step, the forms $\kappa_i(t)$ are changing in accordance with the solution of (50). It will, however, be consistent with the original MSCL up to the order of the method.

As was observed in Section 3.1, applying a higher order Lobatto IIIA–IIIB discretization in space only modifies the linear terms of the ODEs. The effect this has on the linear–nonlinear splitting is to modify the operator $L$ such that more stage values are coupled together. The structure of Eqs. (48) and (50) remains unchanged, however the details of evaluating the time-$\Delta t$ map become more complicated.

**3.2.2. 3 term (real–imaginary–nonlinear) splitting.** We can write the two-stage Lobatto pair discretization in terms of the internal stage variables $v_{i+1/2}$ and $w_{i+1/2}$ as follows:

$$\begin{aligned} -\partial_t q_i + \frac{1}{\Delta x}(v_{i+1/2} - v_{i-1/2}) &= -2(p_i^2 + q_i^2)p_i, \\ \partial_t p_i + \frac{1}{\Delta x}(w_{i+1/2} - w_{i-1/2}) &= -2(p_i^2 + q_i^2)q_i, \\ -\frac{1}{\Delta x}(p_{i+1} - p_i) &= -v_{i+1/2}, \\ -\frac{1}{\Delta x}(q_{i+1} - q_i) &= -w_{i+1/2}. \end{aligned} \tag{51}$$

This satisfies the semi-discrete MSCL

$$\partial_t(dp_i \wedge dq_i) + \frac{1}{\Delta x}(dv_{i+1/2} \wedge dp_{i+1} - dv_{i-1/2} \wedge dp_i) + \frac{1}{\Delta x}(dw_{i+1/2} \wedge dq_{i+1} - dw_{i-1/2} \wedge dq_i) = 0. \tag{52}$$

In this splitting (which has been used for the linear Schrödinger equation [26]), the $\mathbf{L}^{(j)}$ matrices and corresponding $S^{(j)}(z)$ potentials are

$$\mathbf{L}^{(1)} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad \mathbf{L}^{(2)} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}, \qquad \mathbf{L}^{(3)} = \mathbf{0}, \tag{53}$$

$S^{(1)}(z) = -\frac{1}{2}v^2$, $S^{(2)}(z) = -\frac{1}{2}w^2$, $S^{(3)}(z) = -\frac{1}{2}(p^2 + q^2)^2$ which yields the following flows.

**Step 1.**

$$\begin{aligned} q_i^{(1)} &= q_i^{(0)} + \frac{\Delta t}{\Delta x}(v_{i+1/2}^{(1)} - v_{i-1/2}^{(1)}), \\ p_i^{(1)} &= p_i^{(0)} \ (v_i^{(1)} = v_i^{(0)}), \\ \frac{1}{\Delta x}(p_{i+1}^{(1)} - p_i^{(1)}) &= v_{i+1/2}^{(1)}, \end{aligned} \tag{54}$$

for which the exact time-$\Delta t$ flow map satisfies

$$dp_i^{(1)} \wedge dq_i^{(1)} = dp_i^{(0)} \wedge dq_i^{(0)} - \frac{\Delta t}{\Delta x}(dv_{i+1/2}^{(1)} \wedge dp_{i+1}^{(1)} - dv_{i-1/2}^{(1)} \wedge dp_i^{(1)}). \tag{55}$$

**Step 2.**

$$\begin{aligned} q_i^{(2)} &= q_i^{(1)}, \\ p_i^{(2)} &= p_i^{(1)} - \frac{\Delta t}{\Delta x}(w_{i+1/2}^{(1)} - w_{i-1/2}^{(1)}), \\ \frac{1}{\Delta x}(q_{i+1}^{(1)} - q_i^{(1)}) &= w_{i+1/2}^{(1)}, \end{aligned} \tag{56}$$

for which the exact time-$\Delta t$ flow map satisfies

$$dp_i^{(2)} \wedge dq_i^{(2)} = dp_i^{(1)} \wedge dq_i^{(1)} - \frac{\Delta t}{\Delta x}(dw_{i+1/2}^{(1)} \wedge dq_{i+1}^{(1)} - dw_{i-1/2}^{(1)} \wedge dq_i^{(1)}). \tag{57}$$

**Step 3.**

$$\begin{aligned} \begin{pmatrix} q_i^{(3)} \\ p_i^{(3)} \end{pmatrix} &= \begin{bmatrix} \cos\alpha_i\Delta t & \sin\alpha_i\Delta t \\ -\sin\alpha_i\Delta t & \cos\alpha_i\Delta t \end{bmatrix} \begin{pmatrix} q_i^{(2)} \\ p_i^{(2)} \end{pmatrix}, \\ \alpha_i &:= 2((q_i^{(2)})^2 + (p_i^{(2)})^2), \end{aligned} \tag{58}$$

for which the exact time-$\Delta t$ flow map satisfies

$$dp_i^{(3)} \wedge dq_i^{(3)} = dp_i^{(2)} \wedge dq_i^{(2)}. \tag{59}$$

Substituting (55) into (57) and the result into (59) yields

$$\begin{aligned} \frac{1}{\Delta t}(dp_i^{(3)} \wedge dq_i^{(3)} - dp_i^{(0)} \wedge dq_i^{(0)}) + \frac{1}{\Delta x}(dv_{i+1/2}^{(1)} \wedge dp_{i+1}^{(1)} - dv_{i-1/2}^{(1)} \wedge dp_i^{(1)}) \\ + \frac{1}{\Delta x}(dw_{i+1/2}^{(1)} \wedge dq_{i+1}^{(1)} - dw_{i-1/2}^{(1)} \wedge dq_i^{(1)}) = 0, \end{aligned} \tag{60}$$

which is a fully discrete, local version of (52). The method is explicit. The method is first order in time; a higher-order composition would have a different MSCL.

## 4. Conservation laws

NLS has three basic conservation laws that can be derived in a unified way from a multisymplectic form of Noether's theorem: energy from the symmetry $t \mapsto t + c$, momentum from the symmetry $x \mapsto x + c$, and norm from the phase symmetry $\psi \mapsto e^{i\theta}\psi$. Discrete versions of these can be preserved if the symmetry is preserved. Spatial discretization by a fixed grid destroys the spatial translation symmetry but not the time or phase symmetries, hence the semi-discrete system (Eq. (19)) has semi-discrete conservation laws for energy and norm but not for momentum. Time discretization destroys the time symmetry; no method will have a fully discrete energy conservation law.

That leaves the norm conservation law, which for the PDE (9) is

$$(q^2 + p^2)_t + (pq_x - qp_x)_x = 0, \tag{61}$$

with associated conserved quantity (subject to suitable boundary conditions) $\int (q^2+p^2)\,\mathrm{d}x$ $(=\|\psi\|_2^2)$. The semi-discrete conservation law associated with Eq. (19) is

$$(q_i^2+p_i^2)_t + \frac{1}{\Delta x^2}\Delta_x^+(p_{i-1}(q_i-q_{i-1}) - q_{i-1}(p_i-p_{i-1})) = 0 \qquad (62)$$

with conserved quantity $\sum_i (q_i^2+p_i^2)$. Here $\Delta_x^+$ is a forward difference in space.

Time discretization by the Lobatto IIIA–IIIB method (Section 3.1) and the real–imaginary splitting (Section 3.2.2) do not preserve the phase symmetry because of the splitting across the $p$–$q$ variables. Those methods therefore do not have a discrete norm conservation law and do not conserve $\sum_i (q_i^2+p_i^2)$. Time discretization by linear–nonlinear splitting (Section 3.2.1) does preserve the phase symmetry. The first (linear) step obeys Eq. (62) exactly, while the second (nonlinear) step obeys $(q_i^2+p_i^2)_t = 0$. Therefore this method has a discrete norm conservation law in the same sense in which it has a discrete multisymplectic conservation law: integrating Eq. (62) and substituting the solution gives a nonlocal conservation law. Such a law is, however, sufficient to conserve $\sum_i (q_i^2+p_i^2)$.

Finally, time discretization by the midpoint rule does preserve the phase symmetry. This method is well known to preserve the total norm; here, we show that it also satisfies a discrete conservation law:

$$\begin{aligned}((q_i^{n+1})^2+(p_i^{n+1})^2) - ((q_i^n)^2+(p_i^n)^2) &= (q_i^{n+1}-q_i^n)(q_i^{n+1}+q_i^n) + (p_i^{n+1}-p_i^n)(p_i^{n+1}+p_i^n)\\ &= \Delta t(2\bar q_i(D^2\bar p_i + 2(\bar q_i^2+\bar p_i^2)\bar p_i) + 2\bar p_i(-D^2\bar q_i - 2(\bar q_i^2+\bar p_i^2)\bar q_i))\\ &= \Delta t\Delta_x^+(\bar p_{i-1}(\bar q_i-\bar q_{i-1}) - \bar q_{i-1}(\bar p_i-\bar p_{i-1})),\end{aligned} \qquad (63)$$

where $D^2$ is the central difference approximation of $\partial_{xx}$. Hence, the midpoint rule conserves $\sum_i (q_i^2+p_i^2)$.

It is striking that the nonlocal and implicit methods have a discrete norm conservation law, while the local and explicit methods do not.

## 5. Postscript on multisymplecticity

The subtle nature of the multisymplecticity of the linear–nonlinear splitting method leads us to consider the following argument regarding the definition of discrete multisymplecticity. Consider any spatial discretization of any PDE in 1 space and 1 time dimension. Let $\omega_i$ be any set of 2-forms (labelled by spatial grid points) depending on any of the dependent variables. Then for any time integrator we can evaluate $\omega_i^{n+1}-\omega_i^n$ on first variations of solutions and express the result in terms of the solution at time level $n$ to get a putative differential conservation law of the form

$$\omega_i^{n+1}-\omega_i^n = \lambda_i^n. \qquad (64)$$

Note that this does not require any Hamiltonian structure on the part of the PDE or the integrator; it is just bookkeeping. Now suppose that the integrator is symplectic in the sense that $\sum_i \omega_i^{n+1} = \sum_i \omega_i^n$. For simplicity, suppose that the boundary conditions are periodic and the grid points are labelled $1,\ldots,M$. Then we have $\sum_{i=1}^M \lambda_i^n = 0$ and can define $\kappa_1^n = 0$, $\kappa_{i+1}^n = \sum_{j=1}^i \lambda_j^n$ to get an (apparently multisymplectic) differential conservation law

$$\omega_i^{n+1}-\omega_i^n = \kappa_{i+1}^n - \kappa_i^n. \qquad (65)$$

Therefore, the possession of a discrete differential conservation law like Eq. (65) does *not* impose any constraints on the dynamics of the method other than total symplecticity. (We did not even assume that the PDE was multisymplectic.) Some other restriction must be imposed if we are to escape the conclusion that all Hamiltonian ODEs and all symplectic maps are multisymplectic.

The catch, of course, is that the forms $\kappa_i^n$ computed in this way will in general depend on all of $z_1^n, \ldots, z_M^n$; the "conservation law" will be completely nonlocal. The continuous MSCL (3) is completely local. The importance of this factor has been noted before; for example, Bridges and Reich [27] state:

> Let us finally consider the non-compact discretization
>
> $$\Delta t^{-1}\mathbf{K}(z_i^{n+1} - z_i^{n-1}) + \Delta x^{-1}\mathbf{L}(z_{i+1}^n - z_{i-1}^n) = 2\nabla_z S(z_i^n).$$
>
> This scheme satisfies a discrete conservation law of symplecticity of the form (23) [our (65)] but would not be called multisymplectic because of the non-compact nature of its spatial and temporal discretizations.

This nonlocality allows parasitic waves that can damage the solution [17] and, if such a scheme is used for an ODE, none of the good long-time behaviour of symplectic integrators is observed. If we define compactness to mean the coupling of as few dependent variables as possible for any consistent discretization of the PDE, then Gaussian Runge–Kutta and pseudo-spectral methods are not compact yet are called multisymplectic [28].

What is needed is a detailed knowledge of the consequences of (discrete or continuous) multisymplecticity for the dynamics. This is what we have for symplecticity, so that we can assess the relative values of symplecticity, pseudosymplecticity, conjugate symplecticity [1], etc., and it is what we have for systems of hyperbolic conservation laws, where discrete conservation laws ensure not just conservation of total mass, energy, and so on, but also allow precise shock capturing.

**Acknowledgments**

This work was supported in part by the Marsden Fund of the Royal Society of New Zealand. We thank Peter Hydon for useful comments. BR would like to thank the CWI, Amsterdam, for their hospitality and Education New Zealand for financial support.

**Appendix A**

Here we prove that Theorem 2.1 holds.

*Proof* To simplify notation, let $\tilde{b}_j \in \{b_j, \hat{b}_j\}$ and $\tilde{a}_{ij} \in \{a_{ij}, \hat{a}_{ij}\}$ depending on the element of $\mathrm{d}Z_j$ it prepends.

$$\begin{aligned}
\kappa_1 - \kappa_0 &= \frac{1}{2}\mathbf{L}\mathrm{d}z_1 \wedge \mathrm{d}z_1 - \frac{1}{2}\mathbf{L}\mathrm{d}z_0 \wedge \mathrm{d}z_0 \\
&= \frac{1}{2}\mathbf{L}\Big(\mathrm{d}z_0 + \Delta x \sum_j \tilde{b}_j \partial_x \mathrm{d}Z_j\Big) \wedge \Big(\mathrm{d}z_0 + \Delta x \sum_i \tilde{b}_i \partial_x \mathrm{d}Z_i\Big) - \frac{1}{2}\mathbf{L}\mathrm{d}z_0 \wedge \mathrm{d}z_0 \\
&= \frac{1}{2}\Delta x\Bigg(\sum_j \mathbf{L}\Big(\tilde{b}_j \partial_x \mathrm{d}Z_j\Big) \wedge \mathrm{d}z_0 + \sum_i \mathbf{L}\mathrm{d}z_0 \wedge \Big(\tilde{b}_i \partial_x \mathrm{d}Z_i\Big)\Bigg) + \frac{1}{2}\Delta x^2 \sum_{i,j} \Big(\mathbf{L}\tilde{b}_j \partial_x \mathrm{d}Z_j\Big) \wedge \Big(\tilde{b}_i \partial_x \mathrm{d}Z_i\Big) \\
&= \frac{1}{2}\Delta x\Bigg(\sum_j \mathbf{L}\Big(\tilde{b}_j \partial_x \mathrm{d}Z_j\Big) \wedge \Big(\mathrm{d}Z_j - \Delta x \sum_i \tilde{a}_{ji} \partial_x \mathrm{d}Z_i\Big) + \sum_i \mathbf{L}\Big(\mathrm{d}Z_i - \Delta x \sum_j \tilde{a}_{ij} \partial_x \mathrm{d}Z_j\Big) \wedge \Big(\tilde{b}_i \partial_x \mathrm{d}Z_i\Big)\Bigg) \\
&\qquad + \frac{1}{2}\Delta x^2 \sum_{i,j} \Big(\mathbf{L}\tilde{b}_j \partial_x \mathrm{d}Z_j\Big) \wedge \Big(\tilde{b}_i \partial_x \mathrm{d}Z_i\Big)
\end{aligned}$$

$$= \frac{1}{2}\Delta x\bigg(\sum_j \mathbf{L}\Big(\tilde{b}_j\partial_x \mathrm{d}Z_j\Big)\wedge \mathrm{d}Z_j + \sum_i \mathbf{L}\mathrm{d}Z_i \wedge \Big(\tilde{b}_i\partial_x\mathrm{d}Z_i\Big)\bigg) + \frac{1}{2}\Delta x^2\sum_{i,j}\bigg( - \mathbf{L}\Big(\tilde{b}_j\partial_x\mathrm{d}Z_j\Big)\wedge\Big(\tilde{a}_{ji}\partial_x\mathrm{d}Z_i\Big)$$

$$- \mathbf{L}\Big(\tilde{a}_{ij}\partial_x\mathrm{d}Z_j\Big)\wedge\Big(\tilde{b}_i\partial_x\mathrm{d}Z_i\Big) + \mathbf{L}\Big(\tilde{b}_j\partial_x\mathrm{d}Z_j\Big)\wedge\Big(\tilde{b}_i\partial_x\mathrm{d}Z_i\Big)\bigg).$$

Since $\mathbf{L}\mathrm{d}z\wedge\mathrm{d}z$ only has terms of the form $\mathrm{d}z^{(1)}\wedge\mathrm{d}z^{(2)}$, we can write

$$\mathbf{L}\tilde{b}_j\partial_x\mathrm{d}Z_j\wedge\tilde{b}_i\partial_x\mathrm{d}Z_i = 2\sum_{\substack{k,l\\ \mathbf{L}_{kl}\neq 0}}\mathbf{L}_{kl}\Big(b_j\partial_x\mathrm{d}Z^{(1)}_{k,j}\wedge\hat{b}_i\partial_x\mathrm{d}Z^{(2)}_{l,i}\Big),$$

where $\mathrm{d}Z^{(1)}_{k,j}$ is the $k$-th entry of $\mathrm{d}Z^{(1)}_j$ and $\mathrm{d}Z^{(2)}_{l,i}$ is the $l$-th entry of $\mathrm{d}Z^{(2)}_i$. Writing $\mathbf{L}\tilde{b}_j\partial_x\mathrm{d}Z_j\wedge\tilde{a}_{ji}\partial_x\mathrm{d}Z_i$ and $\mathbf{L}\tilde{a}_{ij}\partial_x\mathrm{d}Z_j\wedge\tilde{b}_i\partial_x\mathrm{d}Z_i$ in a similar manner and recalling that $b_i\hat{b}_j - b_i\hat{a}_{ij} - \hat{b}_j a_{ji} = 0$ for all $i,j$, we are left with

$$\kappa_1 - \kappa_0 = \frac{1}{2}\Delta x\sum_j\bigg(\mathbf{L}\Big(\tilde{b}_j\partial_x\mathrm{d}Z_j\Big)\wedge\mathrm{d}Z_j + \mathbf{L}\mathrm{d}Z_j\wedge\Big(\tilde{b}_j\partial_x\mathrm{d}Z_j\Big)\bigg).$$

Now, since we have $b_j = \hat{b}_j$ for all $j$ and $\mathbf{L}$ and $\mathbf{K}$ are skew-symmetric, we can write

$$\begin{aligned}
\kappa_1 - \kappa_0 &= \frac{1}{2}\Delta x\sum_j b_j\bigg(\Big(\mathbf{L}\partial_x\mathrm{d}Z_j\Big)\wedge\mathrm{d}Z_j - \mathrm{d}Z_j\wedge\Big(\mathbf{L}\partial_x\mathrm{d}Z_j\Big)\bigg)\\
&= \frac{1}{2}\Delta x\sum_j b_j\bigg(\Big(D_{zz}S(z)\mathrm{d}Z_j - \mathbf{K}\partial_t\mathrm{d}Z_j\Big)\wedge\mathrm{d}Z_j - \mathrm{d}Z_j\wedge\Big(D_{zz}S(z)\mathrm{d}Z_j - \mathbf{K}\partial_x\mathrm{d}Z_j\Big)\bigg)\\
&= -\frac{1}{2}\Delta x\sum_j b_j\bigg(\Big(\mathbf{K}\partial_t\mathrm{d}Z_j\Big)\wedge\mathrm{d}Z_j + \mathbf{K}\mathrm{d}Z_j\wedge\Big(\partial_x\mathrm{d}Z_j\Big)\bigg)\\
&= -\frac{1}{2}\Delta x\sum_j b_j\partial_t\bigg(\Big(\mathbf{K}\mathrm{d}Z_j\Big)\wedge\mathrm{d}Z_j\bigg)\\
&= -\Delta x\sum_j b_j\partial_t\omega_t.
\end{aligned}$$

□

### Appendix B

Here we prove that Theorem 3.1 holds.

*Proof* Using the notation convention that $\mathrm{d}Z^{n,m}_{i,j}$ represents the variable $\mathrm{d}Z$ at the point $((i+c_j)\Delta x, (n+C_m)\Delta t)$ and $\mathrm{d}z^n_i = \mathrm{d}Z^{n,1}_{i,1}$, the left-hand-side of Eq. (33) is

$$\frac{1}{\Delta t}\sum_j b_j(\omega^1_j - \omega^0_j) + \frac{1}{\Delta x}\sum_m B_m(\kappa^m_1 - \kappa^m_0), \tag{1}$$

where

$$\begin{aligned}
\omega^n_j &= \mathrm{d}P^n_{i,j}\wedge\mathrm{d}Q^n_{i,j},\\
\kappa^m_i &= \mathrm{d}V^{n,m}_i\wedge\mathrm{d}P^{n,m}_i + \mathrm{d}W^{n,m}_i\wedge\mathrm{d}Q^{n,m}_i.
\end{aligned}$$

Expanding the components of Eq. (1) gives

$$\frac{1}{\Delta t}\sum_j b_j(\omega_j^1-\omega_j^0)=\frac{1}{2\Delta t}\Big(\mathrm{d}P_{i,1}^{n+1}\wedge\mathrm{d}Q_{i,1}^{n+1}+\mathrm{d}P_{i,2}^{n+1}\wedge\mathrm{d}Q_{i,2}^{n+1}-\mathrm{d}P_{i,1}^{n}\wedge\mathrm{d}Q_{i,1}^{n}-\mathrm{d}P_{i,2}^{n}\wedge\mathrm{d}Q_{i,2}^{n}\Big) \tag{2}$$

and

$$\begin{aligned}\frac{1}{\Delta x}\sum_m B_m(\kappa_1^m-\kappa_0^m)=&\frac{1}{2\Delta x}\left(\mathrm{d}V_{i+1}^{n,1}\wedge\mathrm{d}P_{i+1}^{n,1}+\mathrm{d}W_{i+1}^{n,1}\wedge\mathrm{d}Q_{i+1}^{n,1}-\mathrm{d}V_{i}^{n,1}\wedge\mathrm{d}P_{i}^{n,1}+\mathrm{d}W_{i}^{n,1}\wedge\mathrm{d}Q_{i}^{n,1}\right)\\&+\frac{1}{2\Delta x}\left(\mathrm{d}V_{i+1}^{n,2}\wedge\mathrm{d}P_{i+1}^{n,2}+\mathrm{d}W_{i+1}^{n,2}\wedge\mathrm{d}Q_{i+1}^{n,2}-\mathrm{d}V_{i}^{n,2}\wedge\mathrm{d}P_{i}^{n,2}+\mathrm{d}W_{i}^{n,2}\wedge\mathrm{d}Q_{i}^{n,2}\right).\end{aligned}$$

Now, since

$$\begin{aligned}\mathrm{d}V_{i,1}^{n,m}&=\mathrm{d}V_{i,2}^{n,m}=:\mathrm{d}V_{i,\frac12}^{n,m},\\\mathrm{d}V_{i+1}^{n,m}&=\mathrm{d}V_{i,\frac12}^{n,m}+\frac{\Delta x}{2}\partial_x\mathrm{d}V_{i,2}^{n,m}\end{aligned}$$

and

$$\mathrm{d}P_{i+1}^{n,m}=\mathrm{d}P_{i}^{n,m}+\Delta x\mathrm{d}V_{i,\frac12}^{n,m},$$

we can write

$$\mathrm{d}V_{i+1}^{n,m}=\frac{1}{\Delta x}(\mathrm{d}P_{i+1}^{n,m}-\mathrm{d}P_{i}^{n,m})+\frac{\Delta x}{2}(\partial_t\mathrm{d}Q_{i,2}^{n,m}-(6(P_{i,2}^{n,m})^2+2(Q_{i,2}^{n,m})^2)\mathrm{d}P_{i,2}^{n,m}-4P_{i,2}^{n,m}Q_{i,2}^{n,m}\mathrm{d}Q_{i,2}^{n,m}).$$

Similarly, we can write

$$\mathrm{d}W_{i+1}^{n,m}=\frac{1}{\Delta x}(\mathrm{d}Q_{i+1}^{n,m}-\mathrm{d}Q_{i}^{n,m})+\frac{\Delta x}{2}(-\partial_t\mathrm{d}P_{i,2}^{n,m}-4P_{i,2}^{n,m}Q_{i,2}^{n,m}\mathrm{d}P_{i,2}^{n,m}-(2(P_{i,2}^{n,m})^2+6(Q_{i,2}^{n,m})^2)\mathrm{d}Q_{i,2}^{n,m}).$$

Noting that

$$\begin{aligned}\mathrm{d}Q_{i}^{n,1}&=\mathrm{d}Q_{i}^{n,2}=:\mathrm{d}Q_{i}^{n,\frac12},\\\mathrm{d}Q_{i,2}^{n,\frac12}&=\mathrm{d}Q_{i+1}^{n,\frac12}\text{ and }\mathrm{d}P_{i,2}^{n,m}=\mathrm{d}P_{i+1}^{n,m},\end{aligned}$$

we have that

$$\begin{aligned}\frac{1}{\Delta x}\sum_m B_m(\kappa_1^m-\kappa_0^m)=&\frac{1}{2\Delta x^2}\Bigg(\mathrm{d}P_{i+1}^{n,1}\wedge\mathrm{d}P_{i}^{n,1}+\mathrm{d}P_{i+1}^{n,2}\wedge\mathrm{d}P_{i}^{n,2}-\mathrm{d}P_{i}^{n,1}\wedge\mathrm{d}P_{i-1}^{n,1}\\&-\mathrm{d}P_{i}^{n,2}\wedge\mathrm{d}P_{i-1}^{n,2}+2(\mathrm{d}Q_{i+1}^{n,\frac12}\wedge\mathrm{d}Q_{i}^{n,\frac12}-\mathrm{d}Q_{i}^{n,\frac12}\wedge\mathrm{d}Q_{i-1}^{n,\frac12})\\&+\frac14\Big(\partial_t\mathrm{d}Q_{i+1}^{n,1}\wedge\mathrm{d}P_{i+1}^{n,1}+\partial_t\mathrm{d}Q_{i+1}^{n,2}\wedge\mathrm{d}P_{i+1}^{n,2}-\partial_t\mathrm{d}Q_{i}^{n,1}\wedge\mathrm{d}P_{i}^{n,1}-\partial_t\mathrm{d}Q_{i}^{n,2}\wedge\mathrm{d}P_{i}^{n,2}\\&-(\partial_t\mathrm{d}P_{i+1}^{n,1}+\partial_t\mathrm{d}P_{i+1}^{n,2})\wedge\mathrm{d}Q_{i+1}^{n,\frac12}+(\partial_t\mathrm{d}P_{i}^{n,1}+\partial_t\mathrm{d}P_{i}^{n,2})\wedge\mathrm{d}Q_{i}^{n,\frac12}\Big)\Bigg)\end{aligned}$$

after cancelling terms of the form $\mathrm{d}Z \wedge \mathrm{d}Z$ and $\mathrm{d}P \wedge \mathrm{d}Q + \mathrm{d}Q \wedge \mathrm{d}P$. Furthermore,

$$\begin{aligned}
\partial_t \mathrm{d}Q_i^{n,1} &= \frac{2}{\Delta t}(\mathrm{d}Q_i^{n,\frac{1}{2}} - \mathrm{d}Q_i^n),\\
\partial_t \mathrm{d}Q_i^{n,2} &= \frac{2}{\Delta t}(\mathrm{d}Q_i^{n+1} - \mathrm{d}Q_i^{n,\frac{1}{2}}),\\
(\partial_t \mathrm{d}P_i^{n,1} + \partial_t \mathrm{d}P_i^{n,2}) &= \frac{2}{\Delta t}(\mathrm{d}P_i^{n+1} - \mathrm{d}P_i^n),
\end{aligned}$$

so

$$\begin{aligned}
&\frac{1}{4}\Big(\partial_t \mathrm{d}Q_{i+1}^{n,1} \wedge \mathrm{d}P_{i+1}^{n,1} + \partial_t \mathrm{d}Q_{i+1}^{n,2} \wedge \mathrm{d}P_{i+1}^{n,2} - \partial_t \mathrm{d}Q_i^{n,1} \wedge \mathrm{d}P_i^{n,1} - \partial_t \mathrm{d}Q_i^{n,2} \wedge \mathrm{d}P_i^{n,2}\\
&\qquad - (\partial_t \mathrm{d}P_{i+1}^{n,1} + \partial_t \mathrm{d}P_{i+1}^{n,2}) \wedge \mathrm{d}Q_{i+1}^{n,\frac{1}{2}} + (\partial_t \mathrm{d}P_i^{n,1} + \partial_t \mathrm{d}P_i^{n,2}) \wedge \mathrm{d}Q_i^{n,\frac{1}{2}}\Big)\\
&= \frac{1}{2\Delta t}\Big((\mathrm{d}Q_{i+1}^{n,\frac{1}{2}} - \mathrm{d}Q_{i+1}^n) \wedge \mathrm{d}P_{i+1}^n + (\mathrm{d}Q_{i+1}^{n+1} - \mathrm{d}Q_{i+1}^{n,\frac{1}{2}}) \wedge \mathrm{d}P_{i+1}^{n+1} - (\mathrm{d}Q_i^{n,\frac{1}{2}} - \mathrm{d}Q_i^n) \wedge \mathrm{d}P_i^n\\
&\qquad - (\mathrm{d}Q_i^{n+1} - \mathrm{d}Q_i^{n,\frac{1}{2}}) \wedge \mathrm{d}P_i^{n+1} - (\mathrm{d}P_{i+1}^{n+1} - \mathrm{d}P_{i+1}^n) \wedge \mathrm{d}Q_{i+1}^{n,\frac{1}{2}} + (\mathrm{d}P_i^{n+1} - \mathrm{d}P_i^n) \wedge \mathrm{d}Q_i^{n,\frac{1}{2}}\Big)\\
&= \frac{1}{2\Delta t}\Big(\mathrm{d}P_{i+1}^n \wedge \mathrm{d}Q_{i+1}^n - \mathrm{d}P_{i+1}^{n+1} \wedge \mathrm{d}Q_{i+1}^{n+1} - \mathrm{d}P_i^n \wedge \mathrm{d}Q_i^n + \mathrm{d}P_i^{n+1} \wedge \mathrm{d}Q_i^{n+1}\Big),
\end{aligned}$$

which gives us

$$\begin{aligned}
\frac{1}{\Delta x}\sum_m B_m(\kappa_1^m - \kappa_0^m) =& \frac{1}{2\Delta x^2}\Big(\mathrm{d}P_{i+1}^n \wedge \mathrm{d}P_i^n + \mathrm{d}P_{i+1}^{n+1} \wedge \mathrm{d}P_i^{n+1} - \mathrm{d}P_i^n \wedge \mathrm{d}P_{i-1}^n - \mathrm{d}P_i^{n+1} \wedge \mathrm{d}P_{i-1}^{n+1}\\
&+ 2(\mathrm{d}Q_{i+1}^{n,\frac{1}{2}} \wedge \mathrm{d}Q_i^{n,\frac{1}{2}} - \mathrm{d}Q_i^{n,\frac{1}{2}} \wedge \mathrm{d}Q_{i-1}^{n,\frac{1}{2}})\Big)\\
&+ \frac{1}{2\Delta t}\Big(\mathrm{d}P_{i+1}^n \wedge \mathrm{d}Q_{i+1}^n - \mathrm{d}P_{i+1}^{n+1} \wedge \mathrm{d}Q_{i+1}^{n+1} - \mathrm{d}P_i^n \wedge \mathrm{d}Q_i^n + \mathrm{d}P_i^{n+1} \wedge \mathrm{d}Q_i^{n+1}\Big).
\end{aligned} \tag{3}$$

Combining Eqs. (2) and (3) we obtain

$$\begin{aligned}
\frac{1}{\Delta t}\sum_j b_j(\omega_j^1 - \omega_j^0) + \frac{1}{\Delta x}\sum_m B_m(\kappa_1^m - \kappa_0^m) =& \frac{1}{\Delta t}\left(\mathrm{d}P_i^{n+1} \wedge \mathrm{d}Q_i^{n+1} - \mathrm{d}P_i^n \wedge \mathrm{d}Q_i^n\right)\\
&+ \frac{1}{2\Delta x^2}\Big(\mathrm{d}P_{i+1}^n \wedge \mathrm{d}P_i^n + \mathrm{d}P_{i+1}^{n+1} \wedge \mathrm{d}P_i^{n+1} - \mathrm{d}P_i^n \wedge \mathrm{d}P_{i-1}^n - \mathrm{d}P_i^{n+1} \wedge \mathrm{d}P_{i-1}^{n+1}\\
&+ 2(\mathrm{d}Q_{i+1}^{n,\frac{1}{2}} \wedge \mathrm{d}Q_i^{n,\frac{1}{2}} - \mathrm{d}Q_i^{n,\frac{1}{2}} \wedge \mathrm{d}Q_{i-1}^{n,\frac{1}{2}})\Big).
\end{aligned} \tag{4}$$

Now, the variational equivalent of the last line of Eq. (36) is

$$\begin{aligned}
\mathrm{d}Q_i^{n+1} = \mathrm{d}Q_i^{n,\frac{1}{2}} + \frac{\Delta t}{2}\Big(&\frac{1}{\Delta x^2}(\mathrm{d}P_{i-1}^{n+1} - 2\mathrm{d}P_i^{n+1} + \mathrm{d}P_{i+1}^{n+1})\\
&+ (6(P_i^{n+1})^2 + 2(Q_i^{n,\frac{1}{2}})^2)\mathrm{d}P_i^{n+1} + 4P_i^{n+1}Q_i^{n,\frac{1}{2}}\mathrm{d}Q_i^{n,\frac{1}{2}}\Big).
\end{aligned}$$

Substituting this into Eq. (4) and eliminating terms of the form $\mathrm{d}Z \wedge \mathrm{d}Z$ and $\mathrm{d}P \wedge \mathrm{d}Q + \mathrm{d}Q \wedge \mathrm{d}P$ gives

$$\begin{aligned}\frac{1}{\Delta t}\sum_j b_j(\omega_j^1 - \omega_j^0) + \frac{1}{\Delta x}\sum_m B_m(\kappa_1^m - \kappa_0^m) = {}& (\frac{1}{\Delta t} + 2P_i^{n+1}Q_i^{n,\frac{1}{2}})\mathrm{d}P_i^{n+1} \wedge \mathrm{d}Q_i^{n,\frac{1}{2}} \\ & - (\frac{1}{\Delta t} + 2P_i^n Q_i^{n-1,\frac{1}{2}})\mathrm{d}P_i^{n+1} \wedge \mathrm{d}Q_i^{n-1,\frac{1}{2}} \\ & + \frac{1}{\Delta x^2}\Big((\mathrm{d}P_{i+1}^n + \mathrm{d}P_{i-1}^n) \wedge \mathrm{d}P_i^n + (\mathrm{d}Q_{i+1}^{n,\frac{1}{2}} + \mathrm{d}Q_{i-1}^{n,\frac{1}{2}}) \wedge \mathrm{d}Q_i^{n,\frac{1}{2}}\Big).\end{aligned}$$

Recalling that $\mathrm{d}p_i^n = \mathrm{d}P_{i,1}^{n,1} = \mathrm{d}P_i^n$ and defining $\mathrm{d}q_i^{n+\frac{1}{2}} = \mathrm{d}Q_i^{n,\frac{1}{2}}$, we can finally write

$$\begin{aligned}\frac{1}{\Delta t}\sum_j b_j(\omega_j^1 - \omega_j^0) + \frac{1}{\Delta x}\sum_m B_m(\kappa_1^m - \kappa_0^m) = {}& (\frac{1}{\Delta t} + 2p_i^{n+1}q_i^{n+\frac{1}{2}})\mathrm{d}p_i^{n+1} \wedge \mathrm{d}q_i^{n+\frac{1}{2}} \\ - (\frac{1}{\Delta t} + 2p_i^n q_i^{n-\frac{1}{2}})\mathrm{d}p_i^n \wedge \mathrm{d}q_i^{n-\frac{1}{2}} + \frac{1}{\Delta x^2}\Big(&(\mathrm{d}p_{i+1}^n + \mathrm{d}p_{i-1}^n) \wedge \mathrm{d}p_i^n + (\mathrm{d}q_{i+1}^{n+\frac{1}{2}} + \mathrm{d}q_{i-1}^{n+\frac{1}{2}}) \wedge \mathrm{d}q_i^{n+\frac{1}{2}}\Big),\end{aligned}$$

thus proving Theorem 3.1. □

## References


[1] Hairer, E., Lubich, C. and Wanner, G., 2006 *Geometric Numerical Integration*, second (Springer-Verlag, Berlin).
[2] McLachlan, R. and Quispel, G., 2006, Geometric Integrators for ODEs. *J. Phys. A*, **39**(19), 5251–5285.
[3] Bridges, T. and Reich, S., 2001, Multi-Symplectic Integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity. *Phys. Lett. A*, **284**, 184–193.
[4] Ryland, B.N., 2007, Multisymplectic Integration. PhD thesis, Massey University, Palmerston North, New Zealand (in preparation).
[5] Marsden, J., Patrick, G. and Shkoller, S., 1998, Multisymplectic Geometry, Variational Integrators, and Nonlinear PDEs. *Commun. Math. Phys.*, **199**, 351–395.
[6] Hong, J., Liu, Y., Munthe-Kaas, H. and Zanna, A., 2006, Globally conservative properties and error estimation of a multi-symplectic scheme for Schrödinger equations with variable coefficients. *Appl. Numer. Math.*, **56**(6), 814–843.
[7] Liu, H. and Zhang, K., 2006, Multi-symplectic Runge–Kutta-type methods for Hamiltonian wave equations. *IMA J. Numer. Anal.*, **26**(2), 252–271.
[8] Chen, J.B., 2005, A multisymplectic integrator for the periodic nonlinear Schrödinger equation. *Appl. Math. Comput.*, **170**(2), 1394–1417.
[9] Sun, J.Q., Gu, X.Y. and Ma, Z.Q., 2004, Numerical study of the soliton waves of the coupled nonlinear Schrödinger system. *Phys. D*, **196**(3–4), 311–328.
[10] Sun, J.Q. and Qin, M.Z., 2003, Multi-symplectic methods for the coupled 1D nonlinear Schrödinger system. *Comput. Phys. Comm.*, **155**(3), 221–235.
[11] Chen, J. and Qin, M., 2002, A multisymplectic variational integrator for the nonlinear Schrödinger equation. *Numer. Methods Partial Differential Equations*, **18**, 523–536.
[12] Chen, J., Qin, M. and Tang, Y., 2002, Symplectic and multi-symplectic methods for the nonlinear Schrödinger equation. *Comput. Math. Appl.*, **43**(8–9), 1095–1106.
[13] Islas, A., Karpeev, D. and Schober, C., 2001, Geometric integrators for the nonlinear Schrödinger equation. *J. Comput. Phys.*, **173**(1), 116–148.
[14] Chen, J., 2001, New schemes for the nonlinear Shrödinger equation. *Appl. Math. Comput.*, **124**(3), 371–379.
[15] Berland, H., Owren, B. and Skaflestad, B., 2006, Solving the nonlinear Schrödinger equation using exponential integrators. .
[16] Hardin, R.H. and Tappert, F.D., 1973, Applications of the split-step Fourier method to the numerical solution of nonlinear and variable coefficient wave equations. *SIAM Review*, **15**, 423.
[17] Ascher, U. and McLachlan, R., 2004, Multisymplectic box schemes and the Korteweg-de Vries Equation. *Appl. Numer. Math*, **48**, 255–269.
[18] Hong, J., Liu, Y. and Sun, G., 2005, The multi-symplecticity of partitioned Runge–Kutta methods for Hamiltonian PDEs. *Math. Comput.*, **75**, 167–181.
[19] Jay, L.O., 1996, Symplectic partitioned Runge–Kutta methods for constrained Hamiltonian systems. *SIAM J. Numer. Anal.*, **33**(1), 368–387.
[20] Leimkuhler, B. and Reich, S., 2004 *Simulating Hamiltonian Dynamics* (Cambridge University Press, Cambridge).
[21] Ablowitz, M.J. and Herbst, B.M., 1989, Numerically induced chaos in the nonlinear Schrödinger equation. *Phys. Rev. Lett.*, **62**(18), 2065–2068.
[22] Islas, A. and Schober, C., 2003, Multi-symplectic methods for generalized Schrödinger equations. *Future Generation Computer Systems*, **19**, 403–413.
[23] Ryland, B.N. and McLachlan, R.I., 2007, On multisymplecticity of partitioned Runge–Kutta methods. (In preparation).
[24] McLachlan, R.I. and Quispel, G.R.W., 2002, Splitting Methods. *Acta Numerica*, pp. 341–434.
[25] Frank, J., 2004, Geometric space-time integration of ferromagnetic materials. *Applied Numerical Mathematics*, **48**, 307–322.
[26] Gray, S. and McLachlan, R.I., 1997, Optimal stability polynomials for splitting methods, with application to the time-dependent Schröder equation. *Appl. Numer. Anal.*, **25**, 275–286.
[27] Bridges, T. and Reich, S., 2006, Numerical methods for Hamiltonian PDEs. *J. Phys. A*, **39**, 5287–5320.

[28] Bridges, T. and Reich, S., 2001, Multi-symplectic spectral discretizations for the Zakharov-Kuznetsov and shallow water equations. *Physica D*, **152**, 491–504.