Geometric Space-Time Integration of Ferromagnetic Materials

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Abstract

The Landau-Lifshitz equation (LLE) governing the flow of magnetic spin in a ferromagnetic material is a PDE with a noncanonical Hamiltonian structure. In this paper we derive a number of new formulations of the LLE as a partial differential equation on a multisymplectic structure. Using this form we show that the standard central spatial discretization of the LLE gives a semi-discrete multisymplectic PDE, and suggest an efficient symplectic splitting method for time integration. Furthermore we introduce a new space-time box scheme discretization which satisfies a discrete local conservation law for energy flow, implicit in the LLE, and made transparent by the multisymplectic framework.

Key words: ferromagnetic materials, Landau-Lifshitz equation, multisymplectic structure, geometric integration

1 Hamiltonian structure of the Landau-Lifshitz equation

This paper addresses the Landau-Lifshitz equation (LLE) as a nonlinear wave equation supporting solitons and stable magnetic vortices, as considered e.g. in [5,20,24]. The LLE governs the flow of magnetic spin in a ferromagnetic material. At a point $\mathbf{x} \in \mathrm{R}^d$ the *spin* $\mathbf{m}(\mathbf{x}, t) = (m_1, m_2, m_3)^T$ in Cartesian coordinates satisfies

$$\mathbf{m}_t = \mathbf{m} \times [\Delta \mathbf{m} + D\mathbf{m} + \mathbf{\Omega}], \tag{1}$$

where Δ is the Laplacian operator in R^d, $D = \mathrm{diag}(d_1, d_2, d_3)$ models anisotropy in the material, and $\mathbf{\Omega}$ is an external magnetic field.

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In applications in micromagnetics, the LLE may additionally include a non-local term, a spin magnitude-preserving Gilbert damping term, as well as a coupling terms to a dynamic external field governed by Maxwell's equations, see [6].

The LLE can be written in the form of a Hamiltonian PDE with a nonlinear Lie-Poisson structure (see e.g. [23,8]). The general form of a Hamiltonian PDE is

$$\mathbf{y}_t = B(\mathbf{y})\frac{\delta H}{\delta \mathbf{y}}, \tag{2}$$

where $\mathbf{y}(\mathbf{x},t) \in \mathrm{R}^p$, H is a functional, $\frac{\delta H}{\delta \mathbf{y}}$ is the vector of variational derivatives of H with respect to $\mathbf{y}$, and $B(\mathbf{y})$ is a Poisson structure matrix, i.e. a skew-symmetric matrix operator satisfying the Jacobi identity (see [23]). If $B(\mathbf{y})$ is a Poisson structure matrix, continuous with respect to $\mathbf{y}$, there is a local change of variables $\bar{\mathbf{y}} = \bar{\mathbf{y}}(\mathbf{y})$ such that the structure assumes a canonical form

$$\frac{\delta \bar{\mathbf{y}}}{\delta \mathbf{y}} B(\mathbf{y}) \frac{\delta \bar{\mathbf{y}}}{\delta \mathbf{y}}^T = J = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & I_{p_1} \\ 0 & -I_{p_1} & 0 \end{bmatrix}, \tag{3}$$

where $p = 2p_1 + p_2$ and I_{p_1} is the p_1-dimensional identity matrix. Expressed in the new variables, the Hamiltonian system (2) becomes

$$\bar{\mathbf{y}}_t = J\frac{\delta H(\bar{\mathbf{y}})}{\delta \bar{\mathbf{y}}}.$$

It is obvious from the structure of J that the dependent variables $\bar{y}_1, \ldots, \bar{y}_{p_2}$ are constants of motion for any Hamiltonian H.

For (1) the Hamiltonian functional is the total energy

$$H = \frac{1}{2}\int |\nabla_{\mathbf{x}}\mathbf{m}|^2 + \mathbf{m}\cdot D\mathbf{m} + 2\boldsymbol{\Omega}\cdot\mathbf{m}\, d\mathbf{x}. \tag{4}$$

and the Poisson structure is

$$B(\mathbf{m}) = \widehat{\mathbf{m}} = \begin{bmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{bmatrix}, \tag{5}$$

which is related to the Poisson structure of the free rigid body [17].

If the spin is alternatively represented in the coordinates $\bar{\mathbf{m}} = (m_\ell, m_\theta, m_z)^T$,

$$m_\ell = \sqrt{m_1^2 + m_2^2 + m_3^2}, \quad m_\theta = \tan^{-1}\frac{m_2}{m_1}, \quad m_z = m_3, \tag{6}$$

where $\tan^{-1}$ denotes the angle (m_1, m_2) makes with the m_1 axis, then the Poisson structure takes the canonical form (3) with $p_1 \equiv p_2 \equiv 1$, which shows that the spin length $m_\ell = |\mathbf{m}|$ is a conserved quantity. Indeed, we have

$$\frac{\partial}{\partial t}|\mathbf{m}|^2 = 2\mathbf{m}\cdot\mathbf{m}_t = 2\mathbf{m}\cdot(\mathbf{m}\times\frac{\delta H}{\delta \mathbf{m}}) = 0, \tag{7}$$

for any H; that is, $|\mathbf{m}|^2$ is a Casimir of (5).

The polar coordinates (6) are well defined except for $m_1 = m_2 = 0$, for which the spin is aligned with the m_3 axis. The degenerate case can be treated by defining a local chart with, for example, m_ℓ, $m_y = m_2$ and $m_\phi = \tan^{-1}(m_1/m_3)$. In this paper *we will always assume that locally either m_1 or m_2 is nonzero.* Although this assumption is crucial for the analysis, the numerical methods developed here are globally defined, making no use of local charts.

Assuming D and Ω are independent of t and x, (1) is time- and space-translation invariant, implying the conservation of the total energy (4) and total momentum (given here for $m_\ell \equiv 1$):

$$P = \int \frac{1}{1+m_3}(m_1\nabla_{\mathbf{x}}m_2 - m_2\nabla_{\mathbf{x}}m_1)\,d\mathbf{x}. \tag{8}$$

Both global invariants are consequences of related local conservation laws. For example, in the simplified case: $\{D = I,\ \Omega = 0,\ d = 1\}$, the energy and momentum conservation laws become,

$$e_t + f_x = 0, \quad e = \frac{1}{2}\mathbf{m}\cdot\mathbf{m}_{xx}, \qquad f = \frac{1}{2}(\mathbf{m}_x\cdot\mathbf{m}_t - \mathbf{m}\cdot\mathbf{m}_{xt}), \tag{9}$$

$$a_t + b_x = 0, \quad a = \frac{1}{2}(m_3 m_{\theta x} - m_\theta m_{3x}), \quad b = \frac{1}{2}(m_\theta m_{3t} - m_3 m_{\theta t} - |\mathbf{m}_x|^2). \tag{10}$$

These conservation laws can be integrated over the domain of interest and under appropriate (for example, periodic) boundary conditions, imply the invariance of the total integral. For $\Omega = 0$, (1) is also time-reversible.

In numerical simulations of the Landau-Lifshitz and related equations, it is crucial to preserve the relation (7). A number of strategies for doing so are encountered in the literature. A general numerical integrator cannot be expected to do this automatically, making it necessary to either impose the condition as a constraint, or to repeatedly project the solution onto the constraint manifold [4]. However, a number of results under the heading of "geometric integration" techniques (see [9]) can be used to construct integrators that automatically preserve the spin magnitude. First, it is well known that the class of Gauss-Legendre Runge-Kutta methods preserves any quadratic invariant such as the spin magnitude (and the total energy!). The implicit midpoint method is quite

common in this context; see the work of Monk and Vacus who use a finite element discretization of micromagnetics [21,22]. Second, given that $\mathbf{m}(x,t)$ evolves on the surface of a sphere, one can derive an equivalent formulation of (1) in the Lie-Group SO(3) and apply Lie Group integrators, as in [11,14]. Third, since the spin magnitude is a Casimir of the Poisson matrix (5), any Poisson integrator will conserve it by definition. In [7] time-reversible, energy conserving, and Poisson integrators were compared against standard methods for the lattice Landau-Lifshitz equation.

The use of geometric integrators places an additional constraint on the discrete phase space of the numerical solution, eliminating some of the freedom ordinary methods have to wander away from geometric structures such as invariant manifolds. On the other hand, the Hamiltonian structure discussed above is really associated with purely temporal quantities. For PDEs, this implies that some integrals over space are well-conserved whereas the local character of the PDE is not addressed. For instance, although the total energy and momentum may be nearly conserved under a symplectic integrator, the flow of energy and momentum from one point in space to another due to the implied conservation laws (9) and (10) is masked by integration. Recent activity has focused on spatio-temporal Hamiltonian structure and *multisymplectic* PDEs, which do address such local conservation properties. In this paper we propose a new space-time discretization of the LLE which exactly conserves a discrete analog of the implicit energy conservation law (9). We will focus on the case of one spatial dimension $d \equiv 1$, although most of what is said carries over to higher dimensions as well.

2 Review of linear multisymplectic structure

In this section we review some of the implications of multisymplectic structure in the case of linear symplectic forms. In the subsequent section we will generalize these ideas to the nonlinear Poisson case of the Landau-Lifshitz equation. For a full discussion of multisymplectic geometry, see the papers of Bridges [1,2] and Marsden [15].

Given a variational description of a continuous dynamical system (see, e.g. Lanczos [12])

$$0 = \delta \iint \mathcal{L}(u, u_t, u_x)\, dt\, dx,$$

the equation of motion is formally given by

$$-\partial_t \frac{\partial \mathcal{L}}{\partial u_t} - \partial_x \frac{\partial \mathcal{L}}{\partial u_x} + \frac{\partial \mathcal{L}}{\partial u} = 0. \tag{11}$$

The corresponding Hamiltonian description introduces a conjugate variable v

related to the temporal derivative u_t by

$$v \equiv \frac{\partial \mathcal{L}}{\partial u_t}, \tag{12}$$

which we assume to define an invertible relationship $u_t = u_t(v)$. Then the Hamiltonian is defined via a Legendre transformation

$$H(u, v) = \int v u_t(v) - \mathcal{L}(u, u_t(v), u_x)\, dx.$$

The variational derivatives of H are prescribed to satisfy the original equation of motion (11) and the definition of the conjugate variable v:

$$\begin{aligned} \frac{\delta H}{\delta u} &= \partial_x \frac{\partial \mathcal{L}}{\partial u_x} - \frac{\partial \mathcal{L}}{\partial u} = -\partial_t v \\ \frac{\delta H}{\delta v} &= u_t(v) + v u_t'(v) - \frac{\partial \mathcal{L}}{\partial u_t} u_t'(v) = \partial_t u, \end{aligned}$$

or, with $\mathbf{y} = (u, v)^T$,

$$J \mathbf{y}_t = \frac{\delta H}{\delta \mathbf{y}}, \qquad J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{13}$$

A space-time analog of this procedure yields a multisymplectic structure as follows [1]. A second conjugate variable w is introduced, this time with respect to the spatial derivative u_x:

$$w \equiv \frac{\partial \mathcal{L}}{\partial u_x}. \tag{14}$$

Again we assume this to define an invertible relation $u_x = u_x(w)$, and a new Hamiltonian is defined by a Legendre transformation with respect to both v and w:

$$S(u, v, w) = v u_t + w u_x - \mathcal{L}(u, u_t(v), u_x(w)).$$

The partial derivatives of S with respect to (u, v, w) are prescribed to satisfy the equation of motion (11) as well as the definitions of v (12) and w (14):

$$\begin{aligned} \frac{\partial S}{\partial u} &= -\frac{\partial \mathcal{L}}{\partial u} = -\partial_t v - \partial_x w \\ \frac{\partial S}{\partial v} &= u_t(v) + v u_t'(v) - \frac{\partial \mathcal{L}}{\partial u_t} u_t'(v) = \partial_t u, \\ \frac{\partial S}{\partial w} &= u_t(w) + w u_x'(v) - \frac{\partial \mathcal{L}}{\partial u_x} u_x'(v) = \partial_x u, \end{aligned}$$

resulting in the form, with $\mathbf{z} = (u, v, w)^T$,

$$K \mathbf{z}_t + L \mathbf{z}_x = \frac{\partial S}{\partial \mathbf{z}}, \tag{15}$$

where

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

Equation (15) with K and L skew-symmetric matrices defines a PDE on a multisymplectic structure. The theory of such systems has been developed by Bridges [1] and Marsden et al. [15].

Some immediate consequences of multisymplectic structure are summarized below:

- **Conservation law of symplecticity**. If $d\mathbf{y}$ is a solution of the variational equation associated with (13), then the symplectic two-form is globally conserved: $\partial_t \frac{1}{2} \int d\mathbf{y} \wedge J d\mathbf{y}\, dx = 0$. Analogously, if $d\mathbf{z}$ is a solution of the variational equation associated with (15), a conservation law of symplecticity holds [2]
$$\partial_t \frac{1}{2} d\mathbf{z} \wedge K d\mathbf{z} + \partial_x \frac{1}{2} d\mathbf{z} \wedge L d\mathbf{z} = 0. \tag{16}$$
Integration of this relation over x with appropriate boundary conditions implies the global conservation of symplecticity.
- **Conservation laws of energy and momentum**. Taking the inner product of (13) with $\mathbf{y}_t$ yields conservation of total energy $H_t = 0$ upon integration over space, whereas taking the inner product of (15) with $\mathbf{z}_t$ and $\mathbf{z}_x$ give local conservation laws of energy and momentum, respectively [1].

$$e_t + f_x = 0, \qquad e = \frac{1}{2}\mathbf{z} \cdot L\mathbf{z}_x - S, \qquad f = \frac{1}{2}\mathbf{z}_t \cdot L\mathbf{z} \tag{17}$$

$$a_t + b_x = 0, \qquad a = \frac{1}{2}\mathbf{z}_x \cdot K\mathbf{z}, \qquad b = \frac{1}{2}\mathbf{z} \cdot K\mathbf{z}_t - S. \tag{18}$$

The multisymplectic structure can be generalized to allow $\mathbf{z}$ dependence in K and L, as long as the two-forms associated with $K(\mathbf{z})$ and $L(\mathbf{z})$ are closed, i.e. can be expressed locally as the differentials of one-forms [1,2].

Experience has demonstrated that numerical methods for Hamiltonian systems (13) which take into account the global conservation of total symplecticity and energy exhibit performance superior to standard methods. It is then reasonable to expect that methods which take into account the local conservation laws associated with (15) will also perform well. To this end Marsden and co-workers [15,13] and Reich and co-workers [25,3] have developed multisymplectic numerical methods.

In this paper we determine a multisymplectic structure for the Landau-Lifshitz equation and discuss related numerical discretizations.

3 Multisymplectic structure of the Landau-Lifshitz equation

To follow the derivation in the previous section, we begin with a variational formulation of the Landau-Lifshitz equation. We start with a formulation in the coordinates (6) since this gives multisymplectic structure matrices K and L that are constant, simplifying analysis. However for numerical computations the Cartesian components (m_1, m_2, m_3) are to be preferred, so a constrained multisymplectic structure follows. See [16] for a general framework for constrained multisymplectic theory.

With the spin expressed in the coordinates (6), the canonical equations of motion are

$$\begin{aligned} m_{\ell t} &= 0 \\ m_{\theta t} &= \frac{\delta H}{\delta m_z} \\ m_{zt} &= -\frac{\delta H}{\delta m_\theta}. \end{aligned}$$

where the energy (4) takes the form

$$\begin{aligned} H = \frac{1}{2}\int m_{\theta x}^2(m_\ell^2 - m_z^2) + \frac{(m_\ell m_{\ell x} - m_z m_{zx})^2}{m_\ell^2 - m_z^2} + m_{zx}^2 \\ + d_1 m_\ell^2 \cos^2 m_\theta + d_2 m_\ell^2 \sin^2 m_\theta + d_3 m_z^2 \\ + 2\Omega_1 m_\ell \cos m_\theta + 2\Omega_2 m_\ell \sin m_\theta + 2\Omega_3 m_z \, dx. \end{aligned} \tag{19}$$

Since $m_\ell(x,t) = m_\ell(x,0)$ is constant in time, it will play the role of a parameter in the variational description. Let $h(m_\theta, m_z, m_{\theta x}, m_{zx})$ be the energy density, that is $H = \int h(m_\theta, m_z, m_{\theta x}, m_{zx})\, dx$. Define the action density $\mathcal{L}$ by

$$\mathcal{L}(m_\theta, m_{\theta t}) = m_z m_{\theta t} - h(m_\theta, m_z, m_{\theta x}, m_{zx}). \tag{20}$$

Introducing new conjugate variables

$$\begin{aligned} q_\theta &= \partial\mathcal{L}/\partial m_{\theta x} = -m_{\theta x}(m_\ell^2 - m_z^2), \\ q_z &= \partial\mathcal{L}/\partial m_{zx} = \frac{m_\ell m_z m_{\ell x} - m_\ell^2 m_{zx}}{m_\ell^2 - m_z^2}, \end{aligned}$$

the multisymplectic Hamiltonian S is obtained via the Legendre transforma-

tion

$$\begin{aligned}
S =& m_z m_{\theta t} + q_\theta m_{\theta x} + q_z m_{zx} - \mathcal{L} \\
=& q_\theta m_{\theta x} + q_z m_{zx} + h(m_\theta, m_z, m_{\theta x}, m_{zx}) \\
=& \frac{1}{2}\left[-\frac{q_\theta^2}{m_\ell^2 - m_z^2} - \frac{q_z^2}{m_\ell^2}(m_\ell^2 - m_z^2) + \frac{2 m_\ell m_{\ell x} m_z q_z}{m_\ell^2} + {m_{\ell}}_x^2 \right. \\
& + d_1 m_\ell^2 \cos^2 m_\theta + d_2 m_\ell^2 \sin^2 m_\theta + d_3 m_z^2 \\
& \left. + 2\Omega_1 m_\ell \cos m_\theta + 2\Omega_2 m_\ell \sin m_\theta + 2\Omega_3 m_z \right]
\end{aligned} \tag{21}$$

and has partial derivatives

$$\begin{aligned}
\frac{\delta S}{\delta m_\theta} &= m_\ell^2 (d_2 - d_1) \sin m_\theta \cos m_\theta + m_\ell (\Omega_2 \cos m_\theta - \Omega_1 \sin m_\theta), \\
\frac{\delta S}{\delta m_z} &= \frac{q_z^2 m_z + q_z m_\ell m_{\ell x}}{m_\ell^2} - \frac{m_z q_\theta^2}{(m_\ell^2 - m_z^2)^2} + d_3 m_z + \Omega_3, \\
\frac{\delta S}{\delta q_\theta} &= -\frac{q_\theta}{m_\ell^2 - m_z^2}, \\
\frac{\delta S}{\delta q_z} &= \frac{-q_z(m_\ell^2 - m_z^2) + m_z m_\ell m_{\ell x}}{m_\ell^2}.
\end{aligned}$$

The multisymplectic structure has form (15) in coordinates $\mathbf{z} = (m_\theta, m_z, q_\theta, q_z)^T$ with

$$K = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{22}$$

The two-forms associated with K and L satisfy the conservation law (16).

The energy and momentum conservation laws for the Landau-Lifshitz equation in these coordinates are given by (9) and (10) with

$$\begin{aligned}
e &= S + \frac{1}{2}(q_{\theta x} m_\theta - m_{\theta x} q_\theta + q_{zx} m_z - m_{zx} q_z) \\
f &= -\frac{1}{2}(q_{\theta t} m_\theta - m_{\theta t} q_\theta + q_{zt} m_z - m_{zt} q_z) \\
a &= -\frac{1}{2}(m_{zx} m_\theta - m_{\theta x} m_z) \\
b &= S + \frac{1}{2}(m_{zt} m_\theta - m_{\theta t} m_z).
\end{aligned}$$

For numerical computations, the coordinates (6) are impractical because m_θ is undefined for $m_z = \pm m_\ell$. Alternatively, we can derive a multisymplectic form for the LLE in Cartesian coordinates with a constraint. We rewrite the

action density $\mathcal{L}$ in terms of Cartesian coordinates using (6). To preserve the spin length, we add it as a constraint with Lagrange multiplier Λ

$$\mathcal{L} = m_3 \frac{m_{2t} m_1 - m_{1t} m_2}{m_1^2 + m_2^2} - \frac{1}{2}\left(|\mathbf{m}_x|^2 + \mathbf{m} \cdot D\mathbf{m} + 2\Omega \cdot \mathbf{m}\right) + \Lambda(|\mathbf{m}|^2 - m_\ell^2).$$

Define $q_j = \partial \mathcal{L}/\partial m_{j_x} = -m_{j_x}$, $j = 1, 2, 3$ and the multisymplectic Hamiltonian becomes

$$S(\mathbf{m}, \mathbf{q}) = \frac{1}{2}(|\mathbf{q}|^2 + \mathbf{m} \cdot D\mathbf{m} + 2\Omega \cdot \mathbf{m}) - \Lambda(|\mathbf{m}|^2 - m_\ell^2). \tag{23}$$

The configuration variable $\mathbf{z} = (m_1, m_2, m_3, q_1, q_2, q_3, \Lambda)^T$, and the structure matrices $K(\mathbf{z})$ and L are

$$K(\mathbf{z}) = \begin{bmatrix} K_1(\mathbf{m}) & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad L = \begin{bmatrix} 0 & I_3 & 0 \\ -I_3 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{24}$$

where

$$K_1(\mathbf{m}) = (m_1^2 + m_2^2)^{-1} \begin{bmatrix} 0 & 0 & -m_2 \\ 0 & 0 & m_1 \\ m_2 & -m_1 & 0 \end{bmatrix}.$$

To check the closedness of the symplectic operator $K(\mathbf{z})$, consider the two-form

$$\kappa(\mathbf{U}, \mathbf{V}) = V_3 \tan^{-1} \frac{U_2}{U_1}, \tag{25}$$

Locally determine orthonormal coordinates such that z_1 and z_2 are not both zero, define a one-form $\alpha(\mathbf{z})\mathbf{V} = \kappa(\mathbf{z}, \mathbf{V})$, i.e. $\alpha(\mathbf{z}) = (0, 0, \tan^{-1}[z_2/z_1])$, and check that $K(\mathbf{z})_{ij} = \frac{\partial \alpha_j}{\partial z_i} - \frac{\partial \alpha_i}{\partial z_j}$.

The equations of motion are

$$K_1(\mathbf{m})\mathbf{m}_t + \mathbf{q}_x = D\mathbf{m} + \Omega - 2\Lambda\mathbf{m} \tag{26}$$

$$-\mathbf{m}_x = \mathbf{q} \tag{27}$$

$$0 = |\mathbf{m}(x,t)|^2 - m_\ell(x,0)^2. \tag{28}$$

Premultiplying (26) with $\widehat{\mathbf{m}}$ (cf. 5) gives, for the first term,

$$\mathbf{m} \times K_1(\mathbf{m})\mathbf{m}_t = \begin{pmatrix} \frac{-m_1 m_3 m_{3t} - m_1 m_2 m_{2t} + m_2^2 m_{1t}}{m_1^2 + m_2^2} \\ \frac{-m_2 m_3 m_{3t} - m_2 m_1 m_{1t} + m_1^2 m_{2t}}{m_1^2 + m_2^2} \\ \frac{m_1^2 m_{3t} + m_2^2 m_{3t}}{m_1^2 + m_2^2} \end{pmatrix} = \mathbf{m}_t, \tag{29}$$

where the second equality follows upon substitution of the time derivative of the constraint (28), i.e. $m_1 m_{1t} + m_2 m_{2t} + m_3 m_{3t} = 0$. Furthermore, $\mathbf{m} \times 2\Lambda \mathbf{m} = 0$, and substitution of (27) for $\mathbf{q}$ in (26) gives (1).

In the next section we turn to the numerical approximation of (26)–(28). We would just mention again that although the above formulation requires the use of local coordinate charts to handle the case $m_1 = m_2 = 0$, the methods to be developed in the next two sections are *globally defined*.

4 Standard semi-discretization

Two different approaches to a discrete numerical analog of multisymplectic structure are: that due to Marsden et al. [15,13], which rests on the discretization of the variational formulation, and that due to Reich [25,3], which focuses on the Hamiltonian side. In this paper we will consider the latter approach.

In this section we show that the standard spatial discretization of the LLE gives a semi-discrete multisymplectic PDE. Let us introduce a uniform grid with grid-spacing ξ, $x_i = i\xi$, and approximations $\mathbf{m}^i(t) \approx \mathbf{m}(x_i, t)$, $\mathbf{q}^i(t) \approx \mathbf{q}(x_i, t)$. Also define forward and backward difference operators

$$\delta_x^+ z^i = \frac{z^{i+1} - z^i}{\xi}, \qquad \delta_x^- z^i = \frac{z^i - z^{i-1}}{\xi}.$$

We isolate the spatial derivative terms in (26)–(28) and discretize using symplectic Euler differencing [9] to obtain

$$\delta_x^+ \mathbf{q}^i = D\mathbf{m}^i + \mathbf{\Omega} - 2\Lambda \mathbf{m}^i - K_1(\mathbf{m}^i)\mathbf{m}_t^i \tag{30}$$

$$-\delta_x^- \mathbf{m}^i = \mathbf{q}^i. \tag{31}$$

This system of differential equations satisfies a semi-discrete multisymplectic conservation law extending the result of [25], in which constant K and L were considered. To see this, define $\mathbf{z}^i = (m_1^i, m_2^i, m_3^i, q_1^i, q_2^i, q_3^i, \Lambda^i)^T$, and let $s \in \mathcal{S}^1$ parameterize a closed curve in phase space.

For κ from (25) one finds the identity

$$\partial_t \kappa(\mathbf{z}^i, \mathbf{z}_s^i) = \partial_s \kappa(\mathbf{z}^i, \mathbf{z}_t^i) - \mathbf{z}_s^i \cdot K(\mathbf{z}^i)\mathbf{z}_t^i. \tag{32}$$

Define a discrete two-form $\bar{\lambda}$ associated with the spatial operator L by

$$\bar{\lambda}(\mathbf{z}^{i-1}, \mathbf{z}^i) = \mathbf{m}^{i-1} \cdot \mathbf{q}^i.$$

It is easily checked that

$$\delta_x^+ \bar{\lambda}(\mathbf{z}^{i-1}, \mathbf{z}_s^i) = \partial_s \bar{\lambda}(\mathbf{z}^i, \delta_x^+ \mathbf{z}^i) - \mathbf{z}_s^i \cdot L \delta_x^{\pm} \mathbf{z}^i, \qquad \text{where} \quad \delta_x^{\pm} \mathbf{z}^i = \begin{pmatrix} \delta_x^- \mathbf{m}^i \\ \delta_x^+ \mathbf{q}^i \end{pmatrix}. \tag{33}$$

Summing (32) and (33) and integrating around $\mathcal{S}^1$ gives

$$\begin{aligned} \oint \partial_t \kappa(\mathbf{z}^i, \mathbf{z}_s^i) + \delta_x^+ \bar{\lambda}(\mathbf{z}^{i-1}, \mathbf{z}_s^i)\, ds \\ &= \oint [\kappa(\mathbf{z}^i, \mathbf{z}_t^i) + \bar{\lambda}(\mathbf{z}^i, \delta_x^+ \mathbf{z}^i)]_s - [\mathbf{z}_s^i \cdot K(\mathbf{z}^i) \mathbf{z}_t^i + \mathbf{z}_s^i \cdot L \delta_x^{\pm} \mathbf{z}^i]\, ds \\ &= - \oint \frac{\partial S}{\partial s}\, ds = 0, \end{aligned}$$

which via Stokes theorem yields a semi-discrete conservation law [2].

This spatial discretization also retains a semi-discrete analog of the local energy conservation law (9), namely:

$$e_t^i + \delta_x^+ f^i = 0, \quad e^i = \frac{1}{2}\left(-(\mathbf{u}^i)^2 + \mathbf{m}^i \cdot D\mathbf{m}^i + 2\Omega \cdot \mathbf{m}^i\right), \quad f_i = \mathbf{m}_t^{i-1} \cdot \mathbf{u}^i.$$

For a given temporal discretization, the error in local energy conservation can be estimated by the residue, defined as

$$r^{i,n} = \delta_t^+ e^{i,n} + \delta_x^+ \bar{f}^{i,n}, \quad \bar{f}^{i,n} = \delta_t^+ \mathbf{m}^{i-1,n} \cdot \mathbf{u}^{i,n}. \tag{34}$$

Simply substituting the relation (31) into (30) for $\mathbf{q}^i$, pre-multiplying by $\widehat{\mathbf{m}^i}$ and inserting the time derivative of the constraint $|m_i(t)|^2 = |m_i(0)|^2$ as in (29) gives the semi-discretized equation

$$\mathbf{m}_t^i = \mathbf{m}^i \times \left[\frac{1}{\xi^2}(\mathbf{m}^{i+1} - 2\mathbf{m}^i + \mathbf{m}^{i-1}) + D\mathbf{m}^i + \mathbf{\Omega}\right], \tag{35}$$

which is globally defined. This system (with $\xi = 1$) and its higher dimensional generalizations are referred to as the Lattice Landau-Lifshitz equation [5]. It comprises a Hamiltonian ODE with Hamiltonian

$$H = \frac{1}{2} \sum_i \frac{1}{\xi^2} |\mathbf{m}^{i+1} - \mathbf{m}^i|^2 + \mathbf{m}^i \cdot D\mathbf{m}^i + 2\mathbf{\Omega} \cdot \mathbf{m}^i \tag{36}$$

and a Poisson structure (5) with block-diagonal form

$$B(\mathbf{m}) = \begin{bmatrix} \ddots & & \\ & \widehat{\mathbf{m}^i} & \\ & & \ddots \end{bmatrix}. \tag{37}$$

Symplectic and time-reversible integrators for (35) were considered in [7]. A symplectic integrator for the isotropic case $D = I_3$ was derived by splitting the sum in (36) according to odd and even i, such that the dynamics generated by H_{odd} and H_{even} are exactly solvable. Since the exact flow map is symplectic for any Hamiltonian and the composition of symplectic maps is symplectic, the overall method is symplectic. Such splitting methods can be made symmetric, and higher order methods can be contrived [19]. A more efficient method was also derived, based on even-odd splitting of the domain. The resulting scheme is not symplectic, but time-reversible, and conserves the energy (36) exactly in the isotropic case. Also considered was the implicit midpoint rule (IM), which for this problem is also not symplectic, but is time-reversible and exactly energy conserving. Due to its implicitness, the IM scheme is suitable for use in very fine discretizations, where the explicit methods suffer from a stability restriction on the stepsize.

Another, possibly better, explicit splitting method is based on a three-term splitting of the Hamiltonian into m_1, m_2 and m_3 contributions:

$$H = H_1 + H_2 + H_3, \qquad H_j = \frac{1}{2}\sum_i \frac{1}{\xi^2}(m_j^{i+1} - m_j^i)^2 + d_j(m_j^i)^2 + 2\Omega_j m_j^i.$$

The dynamics generated by H_1, for example, are

$$\partial_t \begin{pmatrix} m_1^i \\ m_2^i \\ m_3^i \end{pmatrix} = \begin{bmatrix} 0 & -m_3^i & m_2^i \\ m_3^i & 0 & -m_1^i \\ -m_2^i & m_1^i & 0 \end{bmatrix} \begin{pmatrix} \frac{\partial H_1}{\partial m_1^i} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{\partial H_1}{\partial m_1^i} m_3^i \\ -\frac{\partial H_1}{\partial m_1^i} m_2^i \end{pmatrix},$$

which is easily solved to give a rotation about the m_1 axis. The dynamics due to H_2 and H_3 are analogous. Let $\Phi_{\tau,j}$ represent the solution operator for the dynamics due to H_j over an interval τ. The symmetric composition method

$$\mathbf{m}^{n+1} = \Phi_{\tau/2,1} \circ \Phi_{\tau/2,2} \circ \Phi_{\tau,3} \circ \Phi_{\tau/2,2} \circ \Phi_{\tau/2,1} \mathbf{m}^n \tag{38}$$

is second order and symplectic [19]. This method has been used by a number of authors to integrate the Euler rigid body equations (see, e.g., [18]). Its main advantages over the methods of [7] are that it is both fast *and* symplectic (though not exactly energy conserving), and it allows a uniform treatment of anisotropy.

To understand how this splitting fits into the multisymplectic framework, define a decomposition $L = L_1 + L_2 + L_3$ of the spatial symplectic operator, with the nonzero components of L_j given by $(L_j)_{j,j+3} = 1 = -(L_j)_{j+3,j}$, and associated symplectic 2-form $\bar{\lambda}_j$. Similarly, let $S_j(\mathbf{z}) = \frac{1}{2}(q_j^2 + d_j m_j^2 + 2\Omega_j m_j) - \Lambda(|\mathbf{m}|^2 - m_\ell^2)$. Then the split flows $K(\mathbf{z}^i)\mathbf{z}_t^i + L_j \delta_x^{\pm} \mathbf{z}^i = S_j(\mathbf{z}^i)$ are solved consecutively and exactly in time, yielding a sequence of semi-discrete

multisymplectic conservation laws

$$\partial_t \kappa(d\mathbf{z}_j^i, d\mathbf{z}_j^i) + \delta_x^+ \bar{\lambda}_j(d\mathbf{z}_j^{i-1}, d\mathbf{z}_j^i) = 0, \qquad j = 1, 2, 3,$$

analogous to (16), where the differential $d\mathbf{z}_j$ solves the variational equation associated with the jth flow. Summing these relations across the grid with periodic boundary conditions shows that each split timestep is globally symplectic, implying that the composite time integrator is globally symplectic, however it is not clear to what extent the composition may be interpreted as a local conservation law of symplecticity in the sense of [3]. There exist splittings that clearly preserve local conservation, but these are restricted to Hamiltonian splittings for which the identity (27) remains intact, which for the LLE essentially means solving the exact dynamics. Besides splitting, other options for obtaining symplectic integrators for the structure (37) include seeking a global transformation to canonical form or Lie group integrators [9]. Recent papers on Lie group integrators for Landau-Lifshitz equations are [11,14].

Instead, in the next section we will drop the requirement of multisymplecticity and focus on the energy conservation law.

5 Box scheme discretization

Bridges and Reich [3] proposed the multisymplectic box scheme and showed that it preserves discrete energy and momentum conservation laws analogous to (9)–(10) for multisymplectic PDEs with quadratic Hamiltonians. For constant symplectic operators K and L, such PDEs are linear. For the LLE the box scheme is no longer symplectic in time, i.e. it is not a Poisson map for the symplectic operator $K(\mathbf{z})$ of (24). However, since the Hamiltonian (23) is quadratic and L is constant, a discrete energy conservation law still holds. The discrete momentum law is also lost due to the nonlinearity of $K(\mathbf{z})$.

Let $\mathbf{z}^{i,n} \approx \mathbf{z}(x_i, t_n)$ and define, for an arbitrary function f, the average and difference operators

$$\mu_x \mathbf{z}^{i,n} = \frac{1}{2}(\mathbf{z}^{i+1,n} + \mathbf{z}^{i,n}), \qquad \delta_x \mathbf{z}^{i,n} = \frac{1}{\xi}(\mathbf{z}^{i+1,n} - \mathbf{z}^{i,n}),$$
$$\mu_t \mathbf{z}^{i,n} = \frac{1}{2}(\mathbf{z}^{i,n+1} + \mathbf{z}^{i,n}), \qquad \delta_t \mathbf{z}^{i,n} = \frac{1}{\tau}(\mathbf{z}^{i,n+1} - \mathbf{z}^{i,n}),$$

all of which mutually commute. Using these definitions, a discrete chain rule

holds for bilinear forms $\beta(\mathbf{v}, \mathbf{w})$:

$$\begin{aligned}
&\beta(\delta_x \mathbf{v}^i, \mu_x \mathbf{w}^i) + \beta(\mu_x \mathbf{v}^i, \delta_x \mathbf{w}^i) \\
&\qquad = \frac{1}{2\xi}[\beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) + \beta(\mathbf{v}^i, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^{i+1}, \mathbf{w}^i) - \beta(\mathbf{v}^i, \mathbf{w}^i) \\
&\qquad\quad + \beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^i, \mathbf{w}^{i+1}) + \beta(\mathbf{v}^{i+1}, \mathbf{w}^i) - \beta(\mathbf{v}^i, \mathbf{w}^i)] \\
&\qquad = \frac{1}{\xi}[\beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^i, \mathbf{w}^i)] \\
&\qquad = \delta_x \beta(\mathbf{v}^i, \mathbf{w}^i). \qquad (39)
\end{aligned}$$

The same relations hold for μ_t and δ_t.

Consider the multisymplectic form with nonconstant temporal symplectic operator and quadratic function $S(\mathbf{z}) = \frac{1}{2}\mathbf{z} \cdot A\mathbf{z}$:

$$K(\mathbf{z})\mathbf{z}_t + L\mathbf{z}_x = A\mathbf{z}.$$

The box scheme discretization for this system is

$$K(\mu_x\mu_t \mathbf{z}^{i,n})\delta_t\mu_x \mathbf{z}^{i,n} + L\delta_x\mu_t \mathbf{z}^{i,n} = A\mu_x\mu_t \mathbf{z}^{i,n}.$$

Computing the inner product of this expression with $\delta_t\mu_x \mathbf{z}^{i,n}$, and using the skew-symmetry of $K(\mathbf{z})$, we obtain

$$\delta_t\mu_x \mathbf{z}^{i,n} \cdot L\delta_x\mu_t \mathbf{z}^{i,n} = \delta_t\mu_x \mathbf{z}^{i,n} \cdot A\mu_x\mu_t \mathbf{z}^{i,n}.$$

The left side of this equation is, using (39) and skew-symmetry of L,

$$\begin{aligned}
\delta_t\mu_x \mathbf{z}^{i,n} \cdot L\mu_t\delta_x \mathbf{z}^{i,n} &= \frac{1}{2}\delta_t(\mu_x \mathbf{z}^{i,n}) \cdot L\mu_t(\delta_x \mathbf{z}^{i,n}) + \frac{1}{2}\mu_x(\delta_t \mathbf{z}^{i,n}) \cdot L\delta_x(\mu_t \mathbf{z}^{i,n}), \\
&= \frac{1}{2}\delta_x(\delta_t \mathbf{z}^{i,n} \cdot L\mu_t \mathbf{z}^{i,n}) - \frac{1}{2}\delta_x\delta_t \mathbf{z}^{i,n} \cdot L\mu_x\mu_t \mathbf{z}^{i,n} \\
&\quad + \frac{1}{2}\delta_t(\mu_x \mathbf{z}^{i,n} \cdot L\delta_x \mathbf{z}^{i,n}) - \frac{1}{2}\mu_x\mu_t \mathbf{z}^{i,n} \cdot L\delta_x\delta_t \mathbf{z}^{i,n}, \\
&= \frac{1}{2}\delta_t(\mu_x \mathbf{z}^{i,n} \cdot L\delta_x \mathbf{z}^{i,n}) + \frac{1}{2}\delta_x(\delta_t \mathbf{z}^{i,n} \cdot L\mu_t \mathbf{z}^{i,n}),
\end{aligned}$$

and the right side is, using (39) and symmetry of A,

$$\delta_t\mu_x \mathbf{z}^{i,n} \cdot A\mu_x\mu_t \mathbf{z}^{i,n} = \frac{1}{2}\delta_t(\mu_x \mathbf{z}^{i,n} \cdot A\mu_x \mathbf{z}^{i,n}).$$

Combining the last two relations gives the desired discrete energy conservation law

$$\delta_t(\mu_x \mathbf{z}^{i,n} \cdot L\delta_x \mathbf{z}^{i,n} - \mu_x \mathbf{z}^{i,n} \cdot A\mu_x \mathbf{z}^{i,n}) + \delta_x(\delta_t \mathbf{z}^{i,n} \cdot L\mu_t \mathbf{z}^{i,n}) = 0. \qquad (40)$$

For the specific case (26)–(28) discretization with the box scheme gives

$$K_1(\mu_t\mu_x\mathbf{m}^{i,n})\delta_t\mu_x\mathbf{m}^{i,n} + \delta_x\mu_t\mathbf{q}^{i,n} = D\mu_t\mu_x\mathbf{m}^{i,n} + \Omega - 2\Lambda\mu_t\mu_x\mathbf{m}^{i,n} \tag{41}$$

$$-\delta_x\mu_t\mathbf{m}^{i,n} = \mu_t\mu_x\mathbf{q}^{i,n} \tag{42}$$

$$0 = |\mu_t\mu_x\mathbf{m}^{i,n}|^2 - m_\ell(x_i + \xi/2, 0)^2. \tag{43}$$

For a numerical implementation of (41)–(43), we premultiply (42) by $\delta_x\mu_x^{-1}$ and substitute into (41) to eliminate $\mathbf{q}^{i,n}$. We then premultiply both sides by $\mu_t\mu_x\widehat{\mathbf{m}^{i,n}}$ and substitute the discrete derivative of (43) as in the continuous case. Because (43) enforces the spin length constraint at $x_i + \xi/2$, we prefer to work with the spatially averaged spin $\bar{\mathbf{m}}^{i,n} = \mu_x\mathbf{m}^{i,n}$, for which the method becomes

$$\delta_t\bar{\mathbf{m}}^{i,n} = \mu_t\bar{\mathbf{m}}^{i,n} \times [(\delta_x\mu_x^{-1})^2\mu_t\bar{\mathbf{m}}^{i,n} + D\mu_t\bar{\mathbf{m}}^{i,n} + \Omega],$$

which is an implicit midpoint update. The operator μ_x^{-1} exists for periodic boundary conditions and number of gridpoints N odd. For N even, μ_x can be inverted up to the alternating grid sequence using the pseudoinverse.

6 Numerical verification

In this section, we provide a preliminary evaluation of the new methods on the basis of numerical experiments.

All numerical experiments utilize the soliton solution to the LLE published by Tjon & Wright [26]. The soliton is defined, for the anisotropic LLE ($D = I$), by

$$m_1(\eta) = \sin\theta(\eta)\cos\phi(\eta), \quad m_2(\eta) = \sin\theta(\eta)\sin\phi(\eta), \quad m_3 = \cos\theta(\eta),$$

where $\eta = x - x_0 - Vt$ and

$$\cos\theta(\eta) = 1 - 2b^2\mathrm{sech}^2(b\sqrt{\omega}\eta), \tag{44}$$

$$\phi(\eta) = \frac{1}{2}V(x - x_0) \pm \tan^{-1}\left[\left(\frac{b^2}{1-b^2}\right)^{1/2}\tanh(b\sqrt{\omega}\eta)\right], \tag{45}$$

and the parameters V, ω, and b satisfy $V^2/(4\omega) = 1 - b^2$. V is the translation speed of the soliton, b determines its size, and the sign $\pm$ in (45) should agree with that of V. With the external magnetic field given by $\mathbf{\Omega} = (0, 0, \Omega_3)^T$, the parameter ω in (44)–(45) satisfies $\omega = \Omega_3 + \omega_0$, with ω_0 determining the relative phase of m_1 and m_2. These equations describe a right-running wave for positive V and a left running wave for negative V. The function $1 - m_3(\eta)$ is a "pulse" centered at $\eta = 0$. The soliton solution is defined on the whole

real line, but we have truncated it and use periodic boundary conditions on a domain of length 48π.

To simulate a two-soliton collision we chose parameters

$$V_1 = 0.5, \quad b_1 = 0.8, \quad V_2 = -0.8, \quad \Omega_3 = \omega_2 = \omega_1,$$

for which $b_2 = 0.28$. The two solitons were initially located at $x_1 = 12\pi$ and $x_2 = 36\pi$.

The LLE was discretized on a grid with N grid points and periodic boundary conditions using the splitting method (38) and the box scheme (41)–(43). The methods were implemented in Matlab, and for the box scheme Newton iterations were done at time level $n+1$ using the Jacobian from time level n, until convergence of the residue to 10^{-13} in the maximum norm.

Figure 1 illustrates the dynamics of the pulse-like component $1 - m_3$ through approximately one period of motion ($[0, 300]$) of the slow soliton, computed using the splitting method at grid resolution $N = 600$.

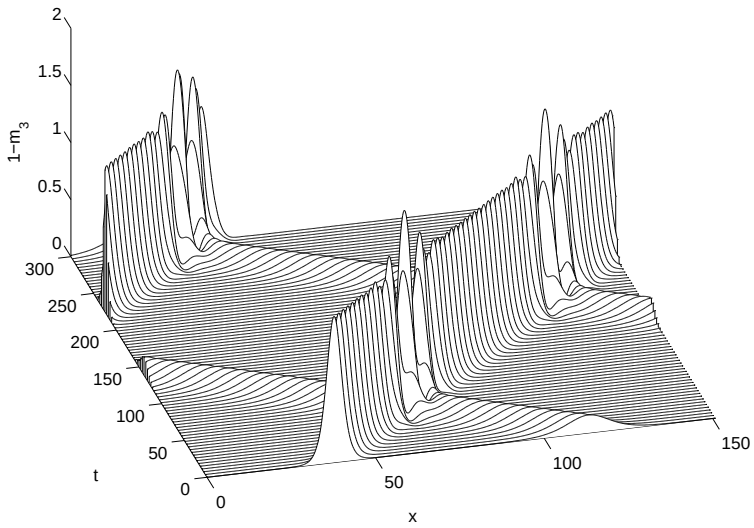

Fig. 1. Collision of two solitons computed with the splitting method ($N = 600$, $\tau = 0.01$).

To more clearly distinguish the features of the two methods, a poorly resolved discretization on $N = 100$ grid points was simulated over the same time interval. Figure 2 illustrates the comparison. The solution obtained with the splitting method exhibits a small lag in group velocity compared to the more accurate solution in Figure 1. The box scheme has a more severe, accelerated group velocity: at the current grid resolution, the slow soliton evolves through approximately 1.5 periods. Comparing the quality of the two solutions, the splitting method is smoother but tends to deteriorate as the integration progresses, and appears to support some small reflected waves emanating from

the collision. With the box scheme, especially the small soliton is very poorly resolved for this grid size, but appears to stabilize before the first collision. No reflections are observed.

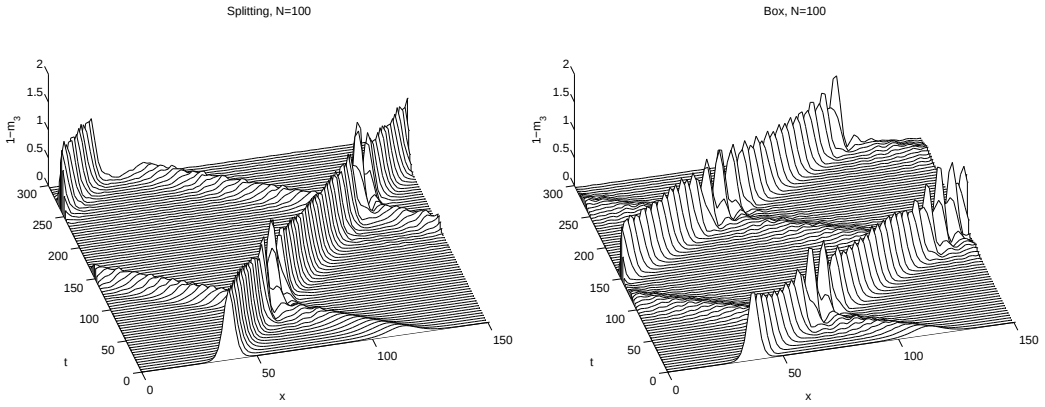

Fig. 2. Collision of two poorly resolved solitons computed with the splitting method (left) and box scheme (right), $N = 100$, $\tau = 0.3$.

We also carried out a long simulation through more than 50 collisions to compare the global conservation properties of the two methods. Using a mesh with $N = 150$, both methods were integrated with $\tau = 0.2$ on an interval $[0, 6000]$. Figure 3 shows the relative changes in total momentum and total energy. Both quantities were well-conserved by the splitting method. For the box scheme the total energy is exactly conserved up to truncation error of the Newton iteration. For the given tolerance (10^{-13}) there is a small drift of magnitude 10^{-11}. Total momentum is not exactly conserved, but the peaks in momentum error with the box scheme are smaller by a factor 10 than those obtained with the splitting method.

The conservation of total energy for the box scheme is a consequence of the exact preservation of the discrete local conservation law (40) under periodic boundary conditions. We also estimate the error in local energy conservation incurred by the splitting method by plotting the absolute value of the residue (34) in Figure 4 for $N = 300$. From the figure it is evident that the residue is largest near the solitons, and that the peaks observed in Figure 3 are accompanied by larger local residues near collisions, but that there are small peaks in the quiescent regions as well. The change in total energy, obtained by summing the $r^{i,n}$ over i, is an order of magnitude smaller than the local quantity due to cancellation of positive and negative contributions. As τ tends to zero, the amplitudes of the peaks in Figure 4 converge to zero.

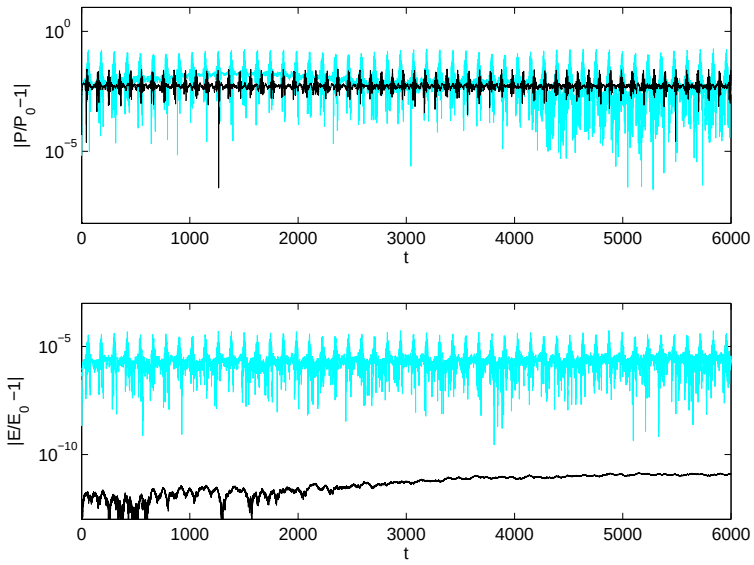

Fig. 3. Relative change in total momentum (top) and total energy (bottom) for a long simulation of 50 soliton collisions, splitting method (gray) and box scheme (black), $N = 150$, $\tau = 0.2$, $T = 6000$.

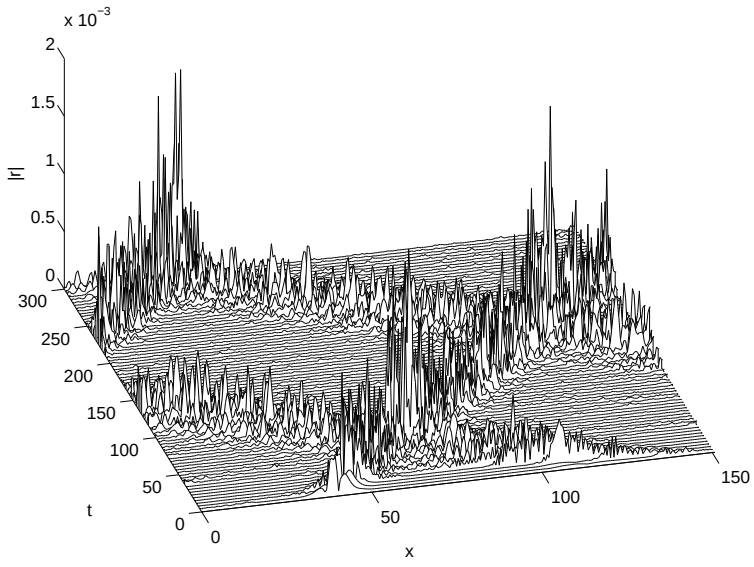

Fig. 4. Residue in local energy conservation law (34) for the splitting method. $N = 300$, $\tau = 0.05$.

7 Conclusions and extensions

In this paper we have generalized the idea of multisymplectic structure to the nonlinear case of the Landau-Lifshitz equation. Motivated by this structure we have proposed a new box scheme discretization which, though not multisymplectic, does retain a discrete energy conservation law. We have also shown that the standard discretization leads to a semi-discrete multisymplectic PDE,

which in turn can be discretized in space using a globally symplectic splitting method.

The methods presented both give good behavior for soliton collisions. The splitting method is globally symplectic and very fast. The box scheme satisfies the discrete analog of the implicit energy conservation law, implying exact global energy conservation, and appears to conserve total momentum better as well. The implications of local energy conservation need to be investigated further.

In micromagnetics applications, the LLE is often coupled with an external field satisfying Maxwell's equations [6]. These equations also have a simple multisymplectic structure, suggesting a unified approach. Maxwell's equations are, for $\mathbf{E}$ the electric field and $\mathbf{B}$ the magnetic induction,

$$\mathbf{B}_t = \nabla \times \mathbf{E}, \qquad -\mathbf{E}_t = \nabla \times \mathbf{B}, \qquad \nabla \cdot \mathbf{B} = \nabla \cdot \mathbf{E} = 0.$$

Writing $\mathbf{z}^T = (\mathbf{E}^T, \mathbf{B}^T)$, Maxwell's equations assume the three-dimensional multisymplectic structure $K\mathbf{z}_t + L^1\mathbf{z}_x + L^2\mathbf{z}_y + L^3\mathbf{z}_z = 0$ with

$$K = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \quad L^j = \begin{bmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{bmatrix}$$

$$\sigma_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Both the box scheme and the symplectic Euler discretization could be applied here, and the box scheme would satisfy discrete conservation laws of symplecticity and energy as well as momenta in 3 directions.

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References

[1] T.J. Bridges, "Multi-symplectic structures and wave propagation", *Math. Proc. Camb. Phil. Soc.* **121** (1997) 147–190.

[2] T.J. Bridges, "A geometric formulation of the conservation of wave action and its implications for signature and the classification of instabilities", *Proc. R. Soc. Lond. A* **453** (1997) 1365–1395.

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

[4] W. E & X.-P. Wang, "Numerical Methods for the Landa-Lifshitz Equation," *SIAM J. Numer. Anal.* **38** (2000) 1647–1665.

[5] L.D. Faddeev & L.A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons*, Springer-Verlag, (1980).

[6] J. Fidler & T. Schrefl, "Micromagnetic modelling—the current state of the art," it J. Phys. D: Appl. Phys. **33** (2000) R135–R156.

[7] J. Frank, W. Huang & B. Leimkuhler, "Geometric integrators for classical spin systems", *J. Comput. Phys.* **133** (1997) 160–172.

[8] E. van Groesen & E.M. de Jager, *Mathematical Structures in Continuous Dynamical Systems*, Studies in Mathematical Physics 6, Elsevier Science, North Holland, (1994).

[9] E. Hairer, C. Lubich & G. Wanner, *Geometric Numerical Integration: Structure Preserving Algorithms for Ordinary Differential Equations*, Springer-Verlag, (2002).

[10] P. Joly & O. Vacus, "Mathematical and numerical studies of nonlinear ferromagnetic materials," *M2AN Math. Model. Numer. Anal.* **33** (1999) 593–626.

[11] P.S. Krishnaprasad & X. Tan, "Cayley transforms in micromagnetics," *Physica B* **306** (2001) 195–199.

[12] C. Lanczos, *The Variational Principles of Mechanics*, 4th edition, Dover, (1986).

[13] A. Lew, J.E. Marsden, M. Ortiz & M. West, "Asynchronous Variational Integrators", preprint, (2002).

[14] D. Lewis & N. Nigam, "Geometric integration on spheres and some interesting applications," J. Comput. Appl. Math. **151** (2003) 141–170.

[15] J.E. Marsden, G.W. Patrick & S. Shkoller, "Multisymplectic geometry, variational integrators, and nonlinear PDEs", *Comm. Math. Phys.* **199** (1999) 351–395.

[16] J.E. Marsden, S. Pekarsky, S. Shkoller & M. West, "Variational Methods, Multisymplectic Geometry and Continuum Mechanics", *J. Geom. Phys.* **38** (2001) 253–284.

[17] J.E. Marsden & T.S. Ratiu, *Introduction to Mechanics and Symmetry*, Springer-Verlag, (1994).

[18] R.I. McLachlan, "Explicit Lie-Poisson integration and the Euler equations," *Phys. Rev. Lett.* **71**, (1993) 3043–3046.

[19] R.I. McLachlan & G.R.W. Quispel, "Splitting methods", *Acta Numerica*, (2002) 341–434.

[20] F.G. Mertens & A.R. Bishop, "Dynamics of Vortices in Two-Dimensional Magnets," in P.L. Christiansen & M.P. Sorensen, eds. *Nonlinear Science at the Dawn of the 21st Century*, Springer, 1999.

[21] P.B. Monk & O. Vacus, "Error Estimates for a Numerical Scheme for Ferrormagnetic Problems," *SIAM J. Numer. Anal.* **36** (1999) 696–718.

[22] P.B. Monk & O. Vacus, "Accurate disctretization of a non-linear micromagnetic problem," *Comput. Methods Appl. Mech. Engrg.* **190** (2001) 5243–5269.

[23] P.J. Olver, *Applications of Lie Groups to Differential Equations*, Springer-Verlag, second edition, (1993).

[24] N. Papanicolaou & P.N. Spathis, "Semitopological solitions in planar ferromagnets," *Nonlinearity* **12** (1999) 285–302.

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

[26] J. Tjon & J. Wright, "Solitons in the continuous Heisenberg spin chain," *Phys. Rev. B* **15** (1977) 3470–3476.