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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.

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1. Hamiltonian structure of the Landau-Lifshitz equation

The Landau-Lifshitz equation (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

$$\mathbf{m}_t = \mathbf{m} \times [\Delta \mathbf{m} + D\mathbf{m} + \mathbf{\Omega}], \tag{1.1}$$

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

The LLE can be written in the form of a Hamiltonian PDE with a nonlinear (i.e. Poisson) structure (see e.g. [15, 6]). The general form of a Hamiltonian PDE is

$$\mathbf{z}_t = B(\mathbf{z}) \frac{\delta H}{\delta \mathbf{z}}, \tag{1.2}$$

where $\mathbf{z}(\mathbf{x}, t) \in \mathrm{R}^p$, H is a functional, $\frac{\delta H}{\delta \mathbf{z}}$ is the vector of variational derivatives of H with respect to $\mathbf{z}$, and $B(\mathbf{z})$ is a Poisson structure matrix, i.e. a skew-symmetric matrix operator satisfying the Jacobi identity (see [15]). If $B(\mathbf{z})$ is a Poisson structure matrix, continuous with respect to $\mathbf{z}$, there is a local change of variables $\bar{\mathbf{z}} = \bar{\mathbf{z}}(\mathbf{z})$ such that the structure assumes a canonical form

$$\frac{\delta \bar{\mathbf{z}}}{\delta \mathbf{z}} B(\mathbf{z}) \frac{\delta \bar{\mathbf{z}}}{\delta \mathbf{z}}^T = J = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & I_{p_1} \\ 0 & -I_{p_1} & 0 \end{bmatrix}, \tag{1.3}$$

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 (1.2) becomes

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

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

For (1.1) the Hamiltonian functional is the total energy

$$H = \frac{1}{2}\int |\nabla_{\mathbf{x}}\mathbf{m}|^2 + \mathbf{m}\cdot D\mathbf{m} + 2\boldsymbol{\Omega}\cdot\mathbf{m}\, d\mathbf{x}. \tag{1.4}$$

and the Poisson structure is

$$B(\mathbf{m}) = [\mathbf{m}\times] = \begin{bmatrix} 0 & -m_3 & m_2 \\ m_3 & 0 & -m_1 \\ -m_2 & m_1 & 0 \end{bmatrix}, \tag{1.5}$$

which is related to the Poisson structure of the free rigid body [12].

If the spin is alternatively represented in the coordinates

$$\bar{\mathbf{m}} = (m_\ell, m_\theta, m_z)^T, \quad m_\ell = \sqrt{m_1^2 + m_2^2 + m_3^2}, \quad m_\theta = \tan^{-1}\frac{m_2}{m_1}, \quad m_z = m_3, \tag{1.6}$$

where $\tan^{-1}$ denotes the angle (m_1, m_2) makes with the m_1 axis, then the Poisson structure takes the canonical form (1.3) 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

$$\frac{\partial}{\partial t}|\mathbf{m}|^2 = 2\mathbf{m}\cdot\mathbf{m}_t = 2\mathbf{m}\cdot(\mathbf{m}\times\frac{\delta H}{\delta \mathbf{m}}) = 0, \tag{1.7}$$

for any H.

The polar coordinates (1.6) 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, $m_y = m_2$ 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.

Other important invariants are the total energy (1.4) and momentum

$$P = \int \frac{1}{1+m_3}(m_1\nabla_{\mathbf{x}}m_2 - m_2\nabla_{\mathbf{x}}m_1)\, d\mathbf{x}. \tag{1.8}$$

As we shall see, both of these global invariants are consequences of related local conservation laws. For example, for the simplified case of an isotropic rod (1D) and no external field, the energy and momentum conservation laws become,

$$e_t + f_x = 0, \quad e = \frac{1}{2}\mathbf{m}\cdot\mathbf{m}_{xx}, \qquad f = \frac{1}{2}(\mathbf{m}_x\cdot\mathbf{m}_t - \mathbf{m}\cdot\mathbf{m}_{xt}), \tag{1.9}$$

$$a_t + b_x = 0, \quad a = \frac{1}{2}(m_3 m_{\theta x} - m_\theta m_{3x}), \quad b = \frac{1}{2}(m_\theta m_{3t} - m_3 m_{\theta t} - |\mathbf{m}_x|^2). \tag{1.10}$$

In numerical simulations of the Landau-Lifshitz and related equations, it is important to preserve the Hamiltonian structure by using symplectic or time reversible integrators. In [5] such "geometric integrators" [7] were compared against standard methods for the lattice Landau-Lifshitz equation. The geometric methods were found to be superior in terms of the preservation of qualitative measures such total energy and spin length conservation (1.7).

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 to 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 (1.9) and (1.10) is masked by integration. Recent activity has focused on spatio-temporal Hamiltonian structure and *multisymplectic* PDEs, in which such local conservation properties *are* addressed. 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 (1.9). 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. PDEs on a multisymplectic structure

Given a variational description of a continuous dynamical system (see, e.g. Lanczos [9])

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

the equation of motion is formally given by

$$-\partial_t \frac{\partial \mathcal{L}}{\partial u_t} - \partial_x \frac{\partial \mathcal{L}}{\partial u_x} + \frac{\partial \mathcal{L}}{\partial u} = 0. \tag{2.1}$$

The corresponding Hamiltonian description defines a conjugate variable v related to the temporal derivative u_t by

$$v \equiv \frac{\partial \mathcal{L}}{\partial u_t}, \tag{2.2}$$

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 (2.1) 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 $\mathbf{z} = (u, v)^T$,

$$J \mathbf{z}_t = \frac{\delta H}{\delta \mathbf{z}}, \qquad J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}. \tag{2.3}$$

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

$$w \equiv \frac{\partial \mathcal{L}}{\partial u_x}. \tag{2.4}$$

Again we assume this to define an invertible relation $u_x = u_x(w)$, then 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 (2.1) as well as the definitions of v (2.2) and w (2.4):

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

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

$$K\mathbf{z}_t + L\mathbf{z}_x = \frac{\partial S}{\partial \mathbf{z}}, \tag{2.5}$$

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 (2.5) 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. [11].

Some immediate consequences of multisymplectic structure are summarized below:

- **Conservation law of symplecticity**. Define symplectic two-forms

$$\kappa(\mathbf{U}, \mathbf{V}) = \frac{1}{2}\mathbf{V} \cdot K\mathbf{U}, \quad \lambda(\mathbf{U}, \mathbf{V}) = \frac{1}{2}\mathbf{V} \cdot L\mathbf{U}. \tag{2.6}$$

  Under the flow of (2.3) total symplecticity κ is conserved $\partial_t \int \kappa \, dx = 0$, whereas under (2.5) a conservation law of symplecticity holds [2]

$$\kappa_t + \lambda_x = 0. \tag{2.7}$$

- **Conservation laws of energy and momentum**. Taking the inner product of (2.3) with $\mathbf{z}_t$ yields conservation of total energy $H_t = 0$ upon integration over space, whereas taking the inner product of (2.5) with $\mathbf{z}_t$ and $\mathbf{z}_x$ give local conservation laws of energy and momentum, respectively [1].

$$e_t + f_x = 0, \qquad e \equiv \frac{1}{2}\mathbf{z} \cdot L\mathbf{z}_x - S, \qquad f \equiv \frac{1}{2}\mathbf{z}_t \cdot L\mathbf{z} \tag{2.8}$$

$$a_t + b_x = 0, \qquad a \equiv \frac{1}{2}\mathbf{z}_x \cdot K\mathbf{z}, \qquad b \equiv \frac{1}{2}\mathbf{z} \cdot K\mathbf{z}_t - S. \tag{2.9}$$

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 (2.3) 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 (2.5) will also perform well. To this end Marsden and co-workers [11, 10] and Reich and co-workers [16, 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. Landau-Lifshitz equation on a multisymplectic structure

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 (1.6) 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.

With the spin expressed in the coordinates (1.6), the canonical equations of motion are

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

where the energy (1.4) becomes

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

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 $h(m_\theta, m_z)$ be the energy density, that is $H = \int h(m_\theta, m_z)\, dx$. Define the action density $\mathcal{L}$ by

$$\mathcal{L}(m_\theta, m_{\theta t}) = m_z m_{\theta t} - h(m_\theta, m_z). \tag{3.1}$$

Introducing new conjugate variables

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

the multisymplectic Hamiltonian S is given by the Legendre transformation

$$\begin{aligned} S =& m_z m_{\theta t} + u_\theta m_{\theta x} + u_z m_{z x} - \mathcal{L} \\ =& u_\theta m_{\theta x} + u_z m_{z x} + h \\ =& \frac{1}{2}\left[-\frac{u_\theta^2}{m_\ell^2 - m_z^2} - \frac{u_z^2}{m_\ell^2}(m_\ell^2 - m_z^2) + \frac{2 m_\ell m_{\ell x} m_z u_z}{m_\ell^2} + m_{\ell x}^2 \right. \\ &\left. + d_1 m_\ell^2 \cos^2 m_\theta + d_2 m_\ell^2 \sin^2 m_\theta + d_3 m_z^2 + 2\Omega_1 m_\ell \cos m_\theta + 2\Omega_2 m_\ell \sin m_\theta + 2\Omega_3 m_z \right], \end{aligned} \tag{3.2}$$

with partial derivatives

$$\begin{aligned} \frac{\delta S}{\delta m_\theta} &= 0, \\ \frac{\delta S}{\delta m_z} &= \frac{u_z^2 m_z + u_z m_\ell m_{\ell x}}{m_\ell^2} - \frac{m_z u_\theta^2}{(m_\ell^2 - m_z^2)^2}, \\ \frac{\delta S}{\delta u_\theta} &= -\frac{u_\theta}{m_\ell^2 - m_z^2}, \\ \frac{\delta S}{\delta u_z} &= \frac{-u_z(m_\ell^2 - m_z^2) + m_z m_\ell m_{\ell x}}{m_\ell^2}. \end{aligned}$$

The multisymplectic structure is defined by (2.5) in coordinates $\mathbf{z} = (m_\theta, m_z, u_\theta, u_z)^T$ with

$$K = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad L = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{3.3}$$

The two-forms associated with K and L, given by (2.6), satisfy the the conservation law (2.7).

The energy and momentum conservation laws for the Landau-Lifshitz equation in these coordinates are given by (1.9) and (1.10) with

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

For numerical computations, the coordinates (1.6) 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 (1.6). 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 $u_j = \partial \mathcal{L} / \partial m_{j_x} = -m_{j_x}$, $j = 1, 2, 3$ and the multisymplectic Hamiltonian becomes

$$S(\mathbf{m}, \mathbf{u}) = \frac{1}{2}(|\mathbf{u}|^2 + \mathbf{m} \cdot D\mathbf{m} + 2\Omega \cdot \mathbf{m}) - \Lambda(|\mathbf{m}|^2 - m_\ell^2). \tag{3.4}$$

The configuration variable $\mathbf{z} = (m_1, m_2, m_3, u_1, u_2, u_3, \Lambda)^T$, and the structure matrices $K(\mathbf{z})$ and L are

$$K(\mathbf{z}) = (m_1^2 + m_2^2)^{-1} \begin{bmatrix} 0 & 0 & -m_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & m_1 & 0 & 0 & 0 & 0 \\ m_2 & -m_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.5}$$

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

$$\kappa(\mathbf{U}, \mathbf{V}) = V_3 \tan^{-1} \frac{U_2}{U_1}. \tag{3.6}$$

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 $K(\mathbf{z})_{ij} = \frac{\partial \alpha_j}{\partial z_i} - \frac{\partial \alpha_i}{\partial z_j}$.

Let us denote the upper left 3×3 block of $K(\mathbf{z})$ in (3.5) by $K_1(\mathbf{m})$. The equations of motion become

$$K_1(\mathbf{m})\mathbf{m}_t + \mathbf{u}_x = D\mathbf{m} + \Omega - 2\Lambda\mathbf{m} \tag{3.7}$$

$$-\mathbf{m}_x = u \tag{3.8}$$

$$0 = |\mathbf{m}(x,t)|^2 - m_\ell(x,0)^2. \tag{3.9}$$

Premultiplying (3.7) with $[\mathbf{m}\times]$ (cf. 1.5) gives, for the first term,

$$\mathbf{m} \times K_1(\mathbf{m})\mathbf{m}_t = (m_1^2 + m_2^2)^{-1} \begin{pmatrix} -m_1 m_3 m_{3t} - m_1 m_2 m_{2t} + m_2^2 m_{1t} \\ -m_2 m_3 m_{3t} - m_2 m_1 m_{1t} + m_1^2 m_{2t} \\ m_1^2 m_{3t} + m_2^2 m_{3t} \end{pmatrix} = \mathbf{m}_t, \tag{3.10}$$

where the final equality follows upon substitution of the time derivative of the constraint (3.9), 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 (3.8) for $\mathbf{u}$ in (3.7) gives (1.1).

In the next section we turn to the numerical approximation of (3.7)–(3.9). 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 the one due to Marsden et al. [11, 10], which rests on the discretization of the variational formulation, and the one due to Reich [16, 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 is symplectic. Let us introduce a uniform grid with grid-spacing ξ, $x_i = i\xi$, and approximations $\mathbf{m}^i(t) \approx \mathbf{m}(x_i, t)$, $\mathbf{u}^i(t) \approx \mathbf{u}(x_i, t)$. Also define forward and backward difference operators

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

We isolate the spatial derivative terms in (3.7)–(3.9) and discretize using symplectic Euler differencing [7] to obtain

$$\delta_x^+ \mathbf{u}^i = D\mathbf{m}^i + \mathbf{\Omega} - 2\Lambda\mathbf{m}^i - K_1(\mathbf{m}^i)\mathbf{m}_t^i \tag{4.1}$$

$$-\delta_x^- \mathbf{m}^i = \mathbf{u}^i. \tag{4.2}$$

This system of differential equations is a semi-discrete multisymplectic PDE [16], and satisfies semi-discrete conservation law. To see this, define $\mathbf{z}^i = (m_1^i, m_2^i, m_3^i, u_1^i, u_2^i, u_3^i, \Lambda^i)^T$, and let $s \in \mathcal{S}^1$ parameterize a closed curve in phase space.

For κ from (3.6) one finds the identity

$$\partial_t \kappa(\mathbf{z}^i, \mathbf{z}_s^i) = \partial_s \kappa(\mathbf{z}^i, \mathbf{z}_t^i) - \mathbf{z}_s^i \cdot K(\mathbf{z}^i)\mathbf{z}_t^i. \tag{4.3}$$

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

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

It is easily checked that

$$\delta_x^+ \bar{\lambda}(\mathbf{z}^{i-1}, \mathbf{z}_s^i) = \partial_s \bar{\lambda}(\mathbf{z}^i, \delta_x^+ \mathbf{z}^i) - \mathbf{z}_s^i \cdot L\delta_x^\pm \mathbf{z}^i, \qquad \text{where} \quad \delta_x^\pm \mathbf{z}^i = \begin{pmatrix} \delta_x^- \mathbf{m}^i \\ \delta_x^+ \mathbf{u}^i \end{pmatrix}. \tag{4.4}$$

Summing (4.3) and (4.4) and integrating around $\mathcal{S}^1$ gives

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

which by Stokes theorem yields a semi-discrete conservation law.

Simply substituting the relation (4.2) into (4.1) for $\mathbf{u}^i$, pre-multiplying by $[\mathbf{m}^i\times]$ and inserting the time derivative of the constraint $|m_i(t)|^2 = |m_i(0)|^2$ as in (3.10) gives the semi-discretized equation

$$\mathbf{m}^i_t = \mathbf{m}^i \times \left[\frac{1}{\xi^2}(\mathbf{m}^{i+1} - 2\mathbf{m}^i + \mathbf{m}^{i-1}) + D\mathbf{m}^i + \mathbf{\Omega}\right], \tag{4.5}$$

which is globally defined. This system (with $\xi \equiv 1$) and its higher dimensional generalizations are referred to as the Lattice Landau-Lifshitz equation [4]. It comprises a Hamiltonian ODE with Hamiltonian

$$H = \frac{1}{2}\sum_i \frac{1}{\xi^2}|\mathbf{m}^{i+1} - \mathbf{m}^i|^2 + \mathbf{m}^i \cdot D\mathbf{m}^i + 2\mathbf{\Omega}\cdot\mathbf{m}^i \tag{4.6}$$

and a Poisson structure (1.5) with block-diagonal form

$$B(\mathbf{z}) = \begin{bmatrix} \ddots & & \\ & [\mathbf{m}^i\times] & \\ & & \ddots \end{bmatrix}. \tag{4.7}$$

Symplectic and time-reversible integrators for (4.5) were considered in [5]. A symplectic integrator for the isotropic case $D = I_3$ was derived by splitting the sum in (4.6) 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 [14]. A more efficient method was also derived, based on even-odd splitting of the domain. The resulting scheme was not symplectic, but time-reversible, and conserved the energy (4.6) 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.

Perhaps a 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

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

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

$$\mathbf{m}^{n+1} = \Phi_{\tau/2,1} \circ \Phi_{\tau/2,2} \circ \Phi_{\tau,3} \circ \Phi_{\tau/2,2} \circ \Phi_{\tau/2,1}\mathbf{m}^n \tag{4.8}$$

is second order and symplectic [14]. This method has been used by a number of authors to integrate the Euler rigid body equations (see, e.g., [13]). Its main advantages over the methods of [5] are that it is fast *and* symplectic, and it allows a uniform treatment of anisotropy.

Although the splitting method (4.8) is symplectic with respect to the temporal symplectic operator $K(\mathbf{z})$, it is not clear that there exists a local conservation law of symplecticity (2.7) in the sense of

[3], because the splitting occurs across the symplectic operator L. In other words it appears that the proposed splitting destroys local conservation. In general there exist splittings which preserve local conservation, but these are restricted to Hamiltonian splittings for which the identity (3.8) remains intact, which for the LLE means essentially solving the exact dynamics. If we exclude splitting, other options for obtaining symplectic integrators for the structure (4.7) include seeking a global transformation to canonical form or Lie group integrators [7]. These options will not be explored here.

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

5. Box scheme discretization

Bridges and Reich [3] proposed the multisymplectic box scheme and showed that it conserves discrete energy and momentum conservation laws 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 (3.5). However, since the Hamiltonian (3.4) 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 $\beta(\mathbf{v}, \mathbf{w})$:

$$\begin{aligned}\beta(\delta_x \mathbf{v}^i, \mu_x \mathbf{w}^i) + \beta(\mu_x \mathbf{v}^i, \delta_x \mathbf{w}^i) =& \frac{1}{2\xi}[\beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) + \beta(\mathbf{v}^i, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^{i+1}, \mathbf{w}^i) - \beta(\mathbf{v}^i, \mathbf{w}^i) \\ &+ \beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^i, \mathbf{w}^{i+1}) + \beta(\mathbf{v}^{i+1}, \mathbf{w}^i) - \beta(\mathbf{v}^i, \mathbf{w}^i)] \\ =& \frac{1}{\xi}[\beta(\mathbf{v}^{i+1}, \mathbf{w}^{i+1}) - \beta(\mathbf{v}^i, \mathbf{w}^i)] \\ =& \delta_x \beta(\mathbf{v}^i, \mathbf{w}^i). \end{aligned} \tag{5.1}$$

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 $K(\mathbf{z})$,

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

The left side of this equation is, using (5.1) and asymmetry of L,

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

and the right side is, using (5.1) 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

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

For the specific case (3.7)–(3.9) discretization with the box scheme gives

$$K_1(\mu_t\mu_x\mathbf{m}^{i,n})\delta_t\mu_x\mathbf{m}^{i,n} + \delta_x\mu_t\mathbf{u}^{i,n} = D\mu_t\mu_x\mathbf{m}^{i,n} + \Omega - 2\Lambda\mu_t\mu_x\mathbf{m}^{i,n} \tag{5.2}$$

$$-\delta_x\mu_t\mathbf{m}^{i,n} = \mu_t\mu_x\mathbf{u}^{i,n} \tag{5.3}$$

$$0 = |\mu_t\mu_x\mathbf{m}^{i,n}|^2 - m_\ell(x_i+\xi/2,0)^2. \tag{5.4}$$

For a numerical implementation of (5.2)–(5.4), we premultiply (5.3) by $\delta_x\mu_x^{-1}$ and substitute into (5.2) to eliminate $\mathbf{u}^{i,n}$. We then premultiply both sides by $[\mu_t\mu_x\mathbf{m}^{i,n}\times]$ and substitute the discrete derivative of (5.4) as in the continuous case. Introducing the spatially averaged spin $\bar{\mathbf{m}}^{i,n} = \mu_x\mathbf{m}^{i,n}$, this system 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.

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 [17]. The soliton is defined by

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

where

$$\cos\theta = 1 - 2b^2\mathrm{sech}^2[b\sqrt{\omega}(x-x_0)], \tag{6.1}$$

$$\phi = \phi_0 + \frac{1}{2}V(x-x_0) + \tan^{-1}\left[\left(\frac{b^2}{1-b^2}\right)^{1/2}\tanh[b\sqrt{\omega}(x-x_0)]\right] \tag{6.2}$$

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. With the external magnetic field given by $\mathbf{\Omega} = (0,0,\Omega_3)^T$, the parameter ω in (6.1)–(6.2) satisfies $\omega = \Omega_3 + \omega_0$, with ω_0 a parameter related to the relative phase of m_1

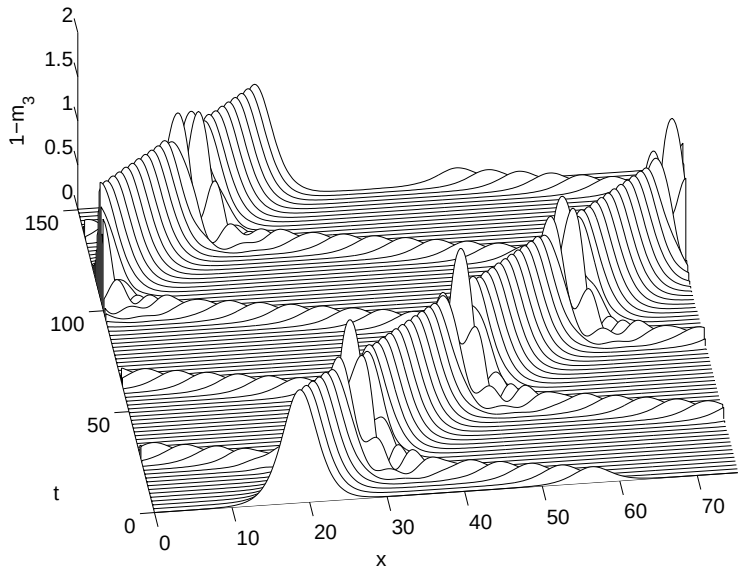

Figure 6.1: Collision of two solitons computed with the box scheme ($N = 321$, $\tau = 0.1463$).

and m_2. These equations describe a right-running wave; a left running wave can be defined by negating the right side of (6.2). Note that only the m_3 component is shape invariant; the function $1 - m_3(x)$ is a "pulse" centered at x_0. The m_1 and m_2 components exhibit harmonic-like motion near x_0. The soliton solution is defined on the whole real line, but we have truncated it and use periodic boundary conditions on a domains of length 24π.

To simulate a two soliton collision we chose parameters

$$V_1 = 0.5, \quad b_1 = 0.5, \quad V_2 = 2, \quad b_2 = 0.3, \quad \Omega_3 = \omega_1.$$

Furthermore, we chose $\phi_2(x)$ to be negative to get a left-running wave.

The LLE was discretized on a grid with N gridpoints and periodic boundary conditions using the splitting method (4.8) and the box scheme (5.2)–(5.4). 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^{-11} in the maximum norm.

Figure 6.1 illustrates the dynamics through approximately one period of the slow soliton, computed with the box scheme (5.2)–(5.4) with grid resolution $N = 321$. The solution obtained with the splitting method is identical to appearance.

To more clearly distinguish the features of the two methods, a poorly resolved discretization on $N = 81$ grid points was simulated. Figure 6.2 contains the comparison. The solution obtained with the splitting method lags slightly behind the more accurate solution in Figure 6.1. With the box scheme, the phase speed is accelerated and the solution is rougher. In our implementation of the box scheme the spatial averaging operator μ_x^{-1} is inverted, which could account for some amplification of high frequency modes.

We also carried out a long simulation through more than 50 collisions on a domain of length 48π to check on the conservation properties of the methods. Figure 6.3 illustrates the results. On the left are the results with the splitting method and on the right those with the box method. The upper plots indicate the amplitude of the m_3 component which is well preserved by both methods throughout the integration. The lower plots show the relative errors in total energy and momentum. Both of these quantities are conserved quite well. For the box scheme the momentum error is approximately an order of magnitude smaller than for the splitting method. Total energy

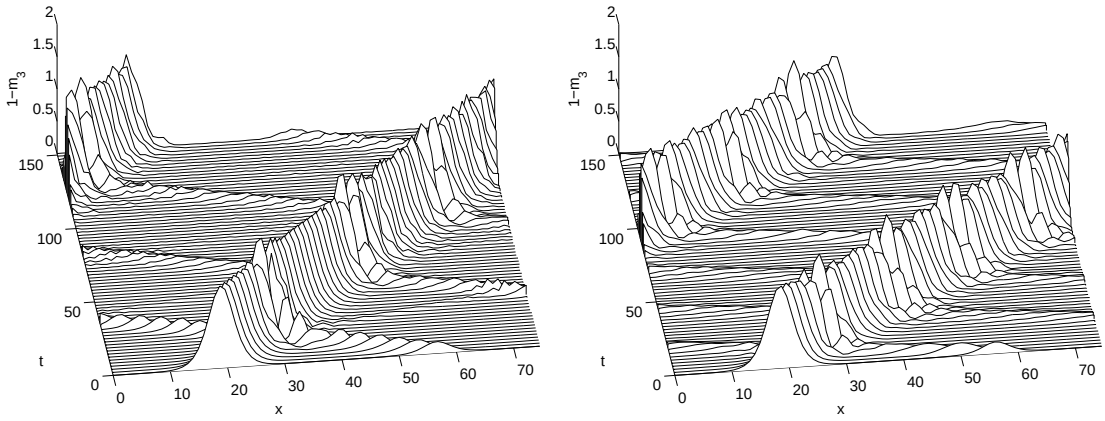

Figure 6.2: Collision of two poorly resolved solitons computed with the splitting method (left) and box scheme (right), $N = 81$, $\tau = 0.2298$.

is exactly conserved by the box scheme with fully converged Newton iterations. For the given tolerance there is a small drift of magnitude 10^{-9}.

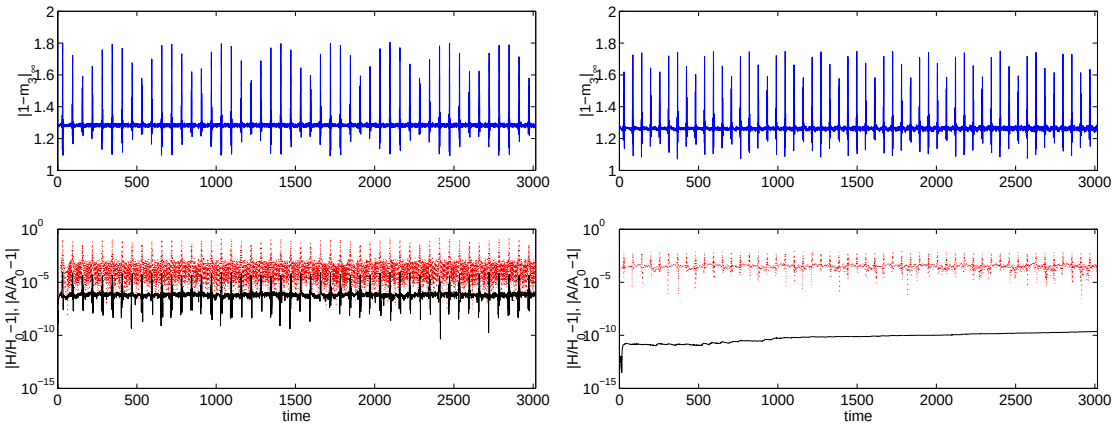

Figure 6.3: Amplitude (above) and relative errors (below) in total energy (solid) and momentum (dotted) through more than 50 soliton collisions, $N = 321$. On the left is the splitting method with time step $\tau = 0.0293$, on the right the box scheme with stepsize $\tau = 0.2927$.

The initial and final positions of the solitons are shown in Figure 6.4 for both methods. Note that although the two methods have different phase speeds so that the final positions of the solitons are different, the discrete solitons are stable solutions even after a relatively long simulation.

7. Conclusions and extensions

The methods presented both give good behavior in the test problems. 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. Also a more efficient implementation of the box scheme is needed.

For a more realistic model, the LLE is often coupled with an external field satisfying Maxwell's equations [8]. These equations also have a simple multisymplectic structure, suggesting a unified

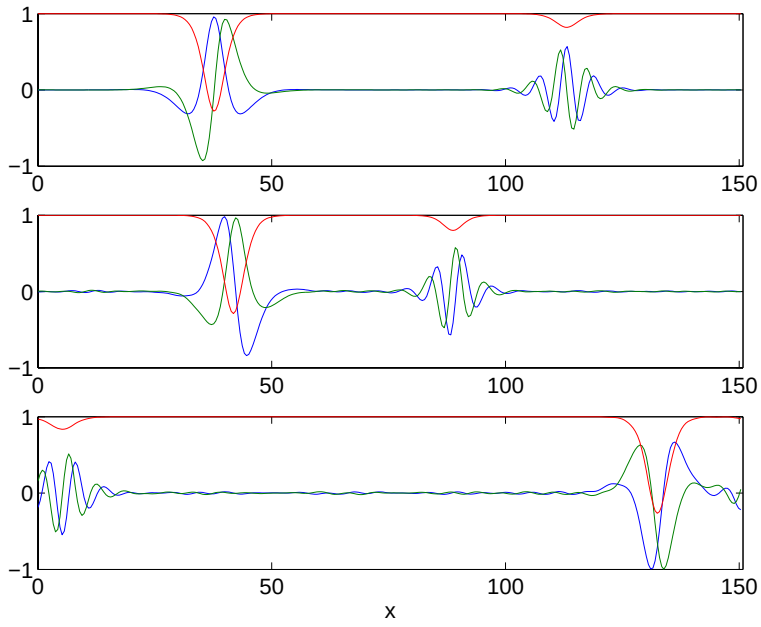

Figure 6.4: Solitons collisions: initial conditions (top), final position after more than 50 collisions, with splitting method (middle) and box scheme (bottom).

approach. Maxwell's equations are, for $\mathbf{E}$ the electric field and $\mathbf{B}$ the magnetic induction,

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

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

$$K = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \quad L^j = \begin{bmatrix} \sigma_j & 0 \\ 0 & \sigma_j \end{bmatrix}, \quad \sigma_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Both the box scheme and the symplectic Euler discretization could be applied here.

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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. L.D. Faddeev & L.A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons*, Springer-Verlag, (1980).
5. J. Frank, W. Huang & B. Leimkuhler, "Geometric integrators for classical spin systems", *J. Comput. Phys.* **133** (1997) 160–172.

6. E. van Groesen & E.M. de Jager, *Mathematical Structures in Continuous Dynamical Systems*, Studies in Mathematical Physics 6, Elsevier Science, North Holland, (1994).
7. E. Hairer, C. Lubich & G. Wanner, *Geometric Numerical Integration: Structure Preserving Algorithms for Ordinary Differential Equations*, Springer-Verlag, (2002).
8. P. Joly & O. Vacus, "Mathematical and numerical studies of nonlinear ferromagnetic materials," *M2AN Math. Model. Numer. Anal.* **33** (1999) 593–626.
9. C. Lanczos, *The Variational Principles of Mechanics*, 4th edition, Dover, (1986).
10. A. Lew, J.E. Marsden, M. Ortiz & M. West, "Asynchronous Variational Integrators", preprint, (2002).
11. J.E. Marsden, G.W. Patrick & S. Shkoller, "Multisymplectic geometry, variational integrators, and nonlinear PDEs", *Comm. Math. Phys.* **199** (1999) 351–395.
12. J.E. Marsden & T.S. Ratiu, *Introduction to Mechanics and Symmetry*, Springer-Verlag, (1994).
13. R.I. McLachlan, "Explicit Lie-Poisson integration and the Euler equations," *Phys. Rev. Lett.* **71**, (1993) 3043–3046.
14. R.I. McLachlan & G.R.W. Quispel, "Splitting methods", *Acta Numerica*, (2002) 341–434.
15. P.J. Olver, *Applications of Lie Groups to Differential Equations*, Springer-Verlag, second edition, (1993).
16. S. Reich, "Multi-symplectic Runge-Kutta collocation methods for Hamiltonian wave equations," *J. Comput. Phys.* **157** (2000) 473–499.
17. J. Tjon & J. Wright, "Solitons in the continuous Heisenberg spin chain," *Phys. Rev. B* **15** (2000) 3470–3476.