COLLECTIVE SYMPLECTIC INTEGRATORS ON $S^2 \times T^* \mathbb{R}^M$

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Abstract. A novel symplectic integrator for Hamiltonian equations on $S^2 \times T^* \mathbb{R}^m$ is developed and studied. Partitioned Runge–Kutta methods for Hamiltonian systems on products of Hamiltonian manifolds are studied, specifically, algebraic conditions for their symplecticity are derived.

1. Introduction

When a differential equation inhibits geometrical properties, it is considered advantageous that numerical approximations to the equation inhibits the same properties. One such geometrical property is the symplecticity inhibited by Hamiltonian systems. In general, a symplectic space is a manifold $M$, equipped with a closed two-form $\omega$. A differential equation

$$\frac{d}{dt} z = X(z),$$

where $X$ is a vector field over $M$, is symplectic if the Lie derivative of $\omega$,

$$\mathcal{L}_X \omega = d\mathbf{i}_X \omega = 0$$

Numerical approximations preserving symplecticity are known as symplectic integrators. Symplectic integrators for ordinary differential equations evolving on vector spaces have been studied by many authors, see for instance [HLW06; SC94] and the references therein.

The situation for non-flat geometries is more complicated, and usually relies on the particular geometry.

This paper studies a special case of non-flat symplectic space, the product of copies of $S^2$ and the canonical symplectic space $T^* \mathbb{R}^M$. This space is of special interest in spin-lattice dynamics.

2. Hamiltonian systems on $S^2 \times T^* \mathbb{R}^m$

Hamiltonian systems evolving on $M = S^2 \times T^* \mathbb{R}^m$ arise in e.g. spin-lattice-electron (SLE) equations. See, e.g. [MWD08; MDW12; Eri+17]. In these systems, each particle $i$ state is given by a position $q_i \in \mathbb{R}^3$, a momentum $p_i \in \mathbb{R}^3$, and a spin $w_i \in S^2$. With $k$ particles, the total state space is thus $S^2_k \times T^* \mathbb{R}^{3k}$.

We write the state of the system $(w, q, p)$, where

$$w = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix} \in S^2_k, \quad p = \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_k \end{bmatrix} \in \mathbb{R}^{3k}, \quad q = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_k \end{bmatrix} \in \mathbb{R}^{3k}.$$
The Hamiltonian for SLE-systems is
\[ H(w, q, p) = T_L(p) + U_L(q) + H_m(w, q) \]
(1)
\[ = \frac{1}{2} \sum_{i=1}^{n} \frac{\|p_i\|^2}{m_i} + U_L(q) - \frac{1}{2} \sum_{i,j=1}^{n} J_{ij}(q)(w_i, w_j) \]
where \( m_i \) is the mass of each individual particle, \( U_L(q) \) is a potential depending on the positions \( q \), and \( J_{ij} \) determines the strength of the spin couplings, depending on the positions \( q \). Typically, \( J_{ij}(q) = J(\|q_i - q_j\|) \), but other functions are possible.

The resulting Hamiltonian equations are
\[ \frac{dq_i}{dt} = \frac{p_i}{m_i} \]
\[ \frac{dp_i}{dt} = -\frac{\partial U_L}{\partial q_i}(q) + \frac{1}{2} \sum_{j,k=1}^{n} \frac{\partial J_{jk}(q)}{\partial q_i} (w_j, w_k) \]
\[ \frac{dw_i}{dt} = w_i \times \left[ \sum_j J_{ij}(q)w_j \right] \]
(2)

For the following, we define the matrix
\[
M = \begin{pmatrix}
  m_1 I_3 \\
  m_2 I_3 \\
  \vdots \\
  m_k I_3
\end{pmatrix}
\]

Symplectic integration of (2) has previously been obtained by splitting methods, see e.g. [OMF01]. These methods rely on a symmetric splitting where each spin is integrated individually. A disadvantage of this approach is that the spins has to be updated in sequence, limiting the possibilities of parallelization. Furthermore, the splitting methods are incapable of handling more general Hamiltonians. For instance, Perera et al. [Per+16] introduce an anisotropy term.

An alternative to the method in the present paper is the method used by Hellsvik et. al. in [Hel+18]

In this article, we suggest a novel approach for symplectic integration on \( S^n \times T^*\mathbb{R}^m \). This approach is based on a partitioned integrator, where the positions and momenta are integrated with a standard symplectic partitioned Runge–Kutta method, and the spins are integrated with a collective symplectic integrator on \( S^n \). The development of symplectic integrators on \( S^n \) is due to by McLachlan, Modin and Verdier [MMV14; MMV15; MMV17].

The novel integrator is implicit, as opposed to splitting-based methods.

The integrators derived in this approach can in principle handle any Hamiltonian on \( S^n \times T^*\mathbb{R}^m \). We will, however, focus on the case where the dependence on the momentum \( p \) can be split of as a quadratic kinetic term \( T_L \).

The geometry needed for these integrators is as follows:

1. The symplectic manifold \( M \) is embedded into a Poisson manifold \( P \), such that the image of \( M \) is a symplectic leaf.

2. \( P \) has a full realization as a canonical symplectic manifold \( N \simeq T^*\mathbb{R}^d \), i.e. there exists an onto Poisson map \( \psi: N \rightarrow P \).
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For the integrators to be well-defined, it is necessary to extend the Hamiltonian $H$ into a function $\bar{H} : \mathbb{P} \rightarrow \mathbb{R}$. This extension is not-unique, however we will fix it to a “canonical” choice, following [MMV17]. The dynamics on the top symplectic manifold $N$ are defined by the pulled-back Hamiltonian $\psi \circ \bar{H}$.

3. SYMPLECTIC AND POISSON STRUCTURES

To proceed, we need to define the various symplectic and Poisson structures involved.

3.1. SYMPLECTIC STRUCTURE ON $M$. Let $M = S \times T^* V$, where $S = S^2_n$ and $V = \mathbb{R}^m$. (In SLD $m = d n$, where $d$ is the dimension of the lattice.) Both $(S, \omega^S)$ and $(T^* V, \omega^V)$ are symplectic manifolds with $\omega^V$ the canonical two-form and

$$\omega^S = \sum_i dA_i,$$

where $A_i$ is the standard area form on the $i$th sphere.

Let $\omega$ be the product symplectic form

$$\omega = \pi_1^* \omega^V + \pi_2^* \omega^S$$

where $\pi_1 : M \rightarrow T^* V$ and $\pi_2 : M \rightarrow S$ are the canonical projections. $(M, \omega)$ is the direct product symplectic manifold of $S$ and $T^* V$.

3.2. POISSON STRUCTURE ON $P$. McLachlan, Modin and Verdier [MMV17] obtained symplectic integrators on $S$ by embedding $S = S^2_n$ as a symplectic leaf in the Poisson manifold $\mathbb{R}^3^n$. A straightforward generalization of this is to embed $M = T^* V \times S$ as a symplectic leaf in a Poisson manifold.

Let $P = T^* V \times \mathbb{R}$, where $\mathbb{R} = \mathbb{R}^3^n$.

$(T^* V, \{\cdot, \cdot\}_V)$ is a Poisson manifold whose Poisson bracket is induced by the symplectic structure,

$$\{f, g\}_V = (\omega^V)^{-1}(df \wedge dg)$$

where $(\omega^V)^{-1}$ is the two-vector obtained by inverting the symplectic form.

The Poisson bracket on $\mathbb{R} = (\mathbb{R}^3)^n$, which we denote $\{\cdot, \cdot\}_S$, is the sum of Poisson brackets on each copy of $\mathbb{R}^3$,

$$\{f, g\}_S(w) = \kappa(w)(df \wedge dg) = \sum_i \left\langle w_i, \left[ \frac{\partial f (w)}{\partial w_i}, \frac{\partial g (w)}{\partial w_i} \right] \right\rangle.$$

On $P$, we obtain a Poisson bracket by taking the sum of the brackets on each component,

$$\{f, g\}(y, w) = (\omega^V)^{-1}(dy f(y, w) \wedge dy g(y, w)) + \kappa(w)(d_w f(y, w) \wedge d_w g(y, w)),$$

for all $y \in T^* V, w \in \mathbb{R}$.

In the above equation, $d_y$ and $d_w$ denote the partial differentials, e.g.

$$d_y f = \sum_i \frac{\partial f}{\partial y_i} dy_i.$$
Using canonical coordinates \( y = (p, q) \), the full form of the Poisson bracket is
\[
\{f, g\}(p, q, w) = \sum_{i=1}^{n} \left( \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) + \sum_{j=1}^{n} \left\langle w_j, \left[ \frac{\partial f}{\partial w_j}, \frac{\partial g}{\partial w_j} \right] \right\rangle.
\]

**Proposition 3.1.** \( M \) is a symplectic leaf in \( P \).

*Proof.* \( S \) is a symplectic leaf in \( \mathbb{R} \) and \( T^* \mathbb{V} \) is a symplectic manifold.

Having embedded \( M \) into \( P \), we also need to extend vector fields on \( M \) to vector fields on \( P \). Taking a leaf from [MMV17], we do this by letting the Hamiltonian and vector fields be constant on rays, i.e. sets of the form \( \{ y, \lambda \circ w : \lambda = (\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^n_+ \} \subset P \), where \( y \in T^* \mathbb{V}, w \in \mathbb{R} \) and \( \lambda \circ w = (\lambda_1 w_1, \ldots, \lambda_n w_n) \).

We define a projection map \( \rho_1 : \mathbb{R} \to S \) by
\[
\rho_1(w_1, w_2, \ldots, w_n) := \left( \frac{w_1}{\|w_1\|}, \ldots, \frac{w_n}{\|w_n\|} \right),
\]
and a projection map \( \rho : P \to M \) by
\[
\rho(y, w) = (y, \rho_1(w))
\]

It is a simple exercise to show that if \( H : M \to \mathbb{R} \) is a Hamiltonian with associated vector field, \( X_H \), then \( \bar{H} = H \circ \rho : P \to \mathbb{R} \) is a Hamiltonian on \( P \) with associated Poisson vector field
\[
X_{\bar{H}}(y, w) = X_H(\rho(y, w)).
\]

We call this vector field the extension of \( X_H \) to \( P \).

Notice that \( X_{\bar{H}} \) is tangent to every symplectic leaf, not only to \( M \).

In particular, for the Hamiltonian of interest (1), the extended Hamiltonian takes the form
\[
\bar{H}(w, p, q) = T_L(p) + H_1(w, q)
\]
where \( H_1(w, q) = U_L(q) + H_m(\rho_1(w), q) \).

### 3.3. Realization of \( P \).

**Definition 3.2.** A realization of a Poisson manifold \( (P, \{\cdot, \cdot\}) \) is a symplectic manifold \( (N, \omega_N) \) together with a Poisson map \( \psi : N \to P \). The realization is called full if it is surjective and canonical if \( N \simeq T^* \mathbb{R}^d \) for some \( d \).

A realization of \( P = (\mathbb{R}^3)^n \times T^* \mathbb{V} \) is obtained by using the Hopf fibration map for each copy of \( \mathbb{R}^3 \).

**Proposition 3.3.** Let \( N = \mathbb{C}^{2n} \times T^* \mathbb{R}^m \), equipped with the canonical symplectic structure. We write a point in \( N \) as \((z_1, z_2, p, q)\) where
\[
z_i = (z_1^i, z_2^i, \ldots, z^n_i), \quad \text{for } i = 1, 2
\]
and \( (p, q) \in T^* \mathbb{R}^m \).

Let a map \( \psi : N \to P \) be defined by
\[
\psi(z_1, z_2, p, q) = (J(z_1, z_2), p, q)
\]
\[
= (J(z_1^1, z_2^1), \ldots, J(z_1^n, z_2^n), p, q),
\]
where \( J : \mathbb{C} \times \mathbb{C} \to \mathbb{R}^3 \) is the Hopf fibration map

\[
J(z_1, z_2) = \frac{1}{4} \begin{pmatrix}
2\Re(z_1 z_2^*) \\
2\Im(z_1 z_2^*) \\
(|z_1|^2 - |z_2|^2)
\end{pmatrix}.
\]

\((N, \psi)\) is a full, canonical realization of \( P \).

Proof. Direct products of Poisson maps are Poisson. \( \psi \) is the product of \( n \) copies of the Hopf fibration and the identity map on \( T^* V \). Finally, the Hopf fibration is Poisson [MR99].

The pull-back of the Hamiltonian (3) has the form

\[
\bar{H} \circ \psi(z, p, q) = T_L(p) + H(z, q) = T_L(p) + H_1(J(z), q)
\]

4. Collective Symplectic Integrators

McLachlan, Modin and Verdier introduced Collective symplectic integrators for integration of Poisson systems. The main idea is to utilize a realization \((N, \psi)\) of the Poisson manifold \( P \) and integrate the vector field of the pulled-back Hamiltonian \( H \circ \psi \) on \( N \), with a symplectic method. We will denote this vector field by \( X_{H \circ \psi} \).

To obtain a symplectic integrator on \( P \) (i.e. Poisson and preserves leaves), it is necessary that the update maps of the integrator maps fibers (of \( \psi \)) to fibers, and that the preimages of leaves are preserved.

In our case \( N = \mathbb{C}^{2n} \times T^* \mathbb{R}^m \simeq T^* \mathbb{R}^{2n} \times T^* \mathbb{R}^m \). We use coordinates \((z, p, q)\) on \( N \) and assume we use a PRK method partitioned into these coordinates (i.e. each of the components \( z, p, q \) are integrated with (possibly different) RK methods.)

Lemma 4.1. A PRK method, when applied to a lifted vector field \( X_{H \circ \psi} \), maps fibers to fibers.

Proof. The group \( U(1)^n \) acts on \( N \) with the following action. Write an element in \( U(1)^n \) as

\[ e^{i\theta} = (e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_n}) \]

where \( \theta_k \in [0, 2\pi] \). The action is given by

\[ e^{i\theta} \cdot (z_1, z_2, p, q) = (e^{i\theta} \odot z_1, e^{i\theta} \odot z_2, p, q) \]

This action is linear and symplectic. Furthermore, it preserves fibers and is transitive on each fiber. As the action is symplectic and preserves fibers, it is a symmetry of the lifted vector field. Since the action is also linear, and only affects one of the components, the \( z \)-component, this symmetry is preserved by the partitioned Runge–Kutta method, and is also a symmetry of the update map. Since the action is transitive on each fiber, we can conclude that the update map maps fibers to fibers. \( \square \)

Lemma 4.2. A PRK method, where the \( z \)-component is integrated with a symplectic RK-method, preserves the preimages of leaves.

Proof. The symplectic leaves in \( P \) are given by \( \|w_j\| = r_j \), for each \( j \). By properties of the Hopf map (4), the preimages in \( N \) are given by

\[ |z_1|^2 + |z_2|^2 = 2r_j \]
for each \( j \), and are invariant under the flow of the lifted vector field. As quadratic invariants, depending only on \( z \), these are preserved by the PRK methods if the \( z \)-method is symplectic.

We are almost ready to state the main theorem, except that we need a result on the symplecticity of Partitioned Runge Kutta methods with three components, where one component, \( z \), corresponds to a symplectic space, and the two remaining components, \( p, q \), correspond to Darboux coordinates of another symplectic space.

The symplecticity of such partitioned methods is interesting in its own right, and the proof of this is presented in Section 5.

**Theorem 4.3.** Assume the system on \( N \) is integrated with a partitioned Runge–Kutta method, where

- \( z \) is integrated with a symplectic Runge–Kutta method.
- \((p, q)\) is integrated with a symplectic partitioned Runge–Kutta method and
- The \( b \)-coefficients of the two methods above coincide.

Then the resulting integrator is symplectic. Furthermore, it descends to a symplectic method on \( P \), and the descended method restricts to a symplectic method on \( M \).

**Proof.** Sufficient conditions are that the “upstairs” integrator on \( M \) [MMV17]

(i) is symplectic.
(ii) maps fibers to fibers.
(iii) preserves preimages of leaves in \( P \).

(i) follows from Theorem 5.3 and the remarks following. (ii) is Lemma 4.1. (iii) is Lemma 4.2.

The method used for the numerical tests is a partitioned method where the \( z \)-variable is integrated with the implicit midpoint method and the \((p, q)\)-variable are integrated with the Störmer–Verlet Scheme. As the midpoint method is a one-stage method, and the Störmer–Verlet method has two stages, it is necessary to use the reducible two stage method with Butcher tableau

\[
\begin{array}{c|cc}
 & 1 & 1 \\
\hline
1 & 1 & \frac{1}{2}
\end{array}
\begin{array}{c|cc}
 & 1 & 1 \\
\hline
1 & 1 & \frac{1}{2}
\end{array}
\begin{array}{c|cc}
 & 1 & 1 \\
\hline
1 & 1 & 2
\end{array}
\]

for the \( z \)-coordinate.

In the following equations describing the integrators, we will use \( p, q, \text{etc.} \) for the values before a step of the integrator, and \( \tilde{p}, \tilde{q}, \text{etc.} \) for the values after a step of the integrator.
The partitioned integrator, applied to the Hamiltonian (5) on \(N\) can, after identifications, be written:

\[
P = p - \frac{h}{2} \frac{\partial H}{\partial q}(q, Z)
\]

\[
Z = z + \frac{h}{4} J_z^{-1} \frac{\partial H}{\partial z}(q, Z) + \frac{h}{4} J_z^{-1} \frac{\partial H}{\partial z}(\tilde{q}, Z)
\]

\[
\dot{p} = P - \frac{h}{2} \frac{\partial H}{\partial q}(\tilde{q}, Z)
\]

\[
\ddot{q} = q + hM^{-1} P
\]

\[
\ddot{z} = z + \frac{h}{2} J_z^{-1} \frac{\partial H}{\partial z}(q, Z) + \frac{h}{2} J_z^{-1} \frac{\partial H}{\partial z}(\tilde{q}, Z).
\]

The \(z\)-variable is integrated with the midpoint method. As shown in [MMV16], this integrator coincides with the spherical midpoint method for ray-constant vector fields (As we have here, cf.(3))

We can thus write the scheme as

\[
P = p - \frac{h}{2} \frac{\partial H_1}{\partial q}(q, W)
\]

\[
W = \rho_1(w + \tilde{w})
\]

\[
\dot{p} = P - \frac{h}{2} \frac{\partial H_1}{\partial q}(\tilde{q}, W)
\]

\[
\ddot{q} = q + hM^{-1} P
\]

\[
\ddot{w} = w + \frac{h}{2} \left[ W, \frac{\partial H_1}{\partial w}(q, W) + \frac{\partial H_1}{\partial w}(\tilde{q}, W) \right]
\]

5. Nonstandard Symplectic partitioned Runge–Kutta methods

For the collective integrators proposed, we integrate a Hamiltonian system where the space is partitioned into a product of two symplectic spaces. We therefore need to establish when a partitioned Runge–Kutta method is symplectic for this partitioning.\(^1\)

The conditions are not specific to our application and are here presented in a more general setting.

We first consider the case when a symplectic manifold is partitioned into \(N\) symplectic spaces, and each component is integrated with a (nonpartitioned) Runge–Kutta method.

Consider an ordinary differential equation of the form

\[
\frac{dy^k}{dt} = f^k(y), \quad k = 1, \ldots, N
\]

where

\[
y = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}
\]

\(^1\)Standard symplectic PRK-methods partition into position and momentum variables
Equation (6) can be numerically integrated by a partitioned Runge–Kutta method with coefficients \(b^k_i, a^k_{ij}\), where \(k = 1, \ldots, N\) and \(i, j = 1, \ldots, s\). When writing down the scheme, we write
\[
\tilde{y} = \begin{bmatrix}
\tilde{y}_1 \\
\vdots \\
\tilde{y}_N
\end{bmatrix}
\]
for the updated variables, and
\[
Y_i = \begin{bmatrix}
Y^i_1 \\
\vdots \\
Y^i_N
\end{bmatrix}, \quad i = 1, \ldots, s
\]
for the stage values.

We are interested in which of these schemes preserve symplectic forms of the type
\[
\omega = \sum_{k=1}^{N} \omega_k = \sum_{k=1}^{N} dy^k \wedge J_k dy^k.
\]
where each \(J_k\) is a \(n_k \times n_k\) skew-symmetric, nonsingular matrix

A standard application of the variational equation (see e.g. [HLW06, Chapter VI.4]) shows that for preserving symplectic forms of the above type it is sufficient that the integrator preserves all first integrals of the form
\[
I(Y) = \sum_{k=1}^{N} I_k(y_k) = \sum_{k=1}^{N} B^k(y_k, y^k),
\]
where each \(B^k\) is a symmetric bilinear function.

**Theorem 5.1.** If the coefficients satisfy that

(i) \(b^k_i b^k_j = b^k_i a^k_{ij} + b^k_j a^k_{ji}\) \quad for all \(i, j, k\) and

(ii) \(b^1_i = b^2_i = \cdots = b^k_i\) \quad for all \(i\).

then the scheme preserves all invariants of the form \(I(Y) = \sum_{k=1}^{N} B^k(y_k, y^k)\).

Another way of stating the assumption in the theorem is that each of the Runge–Kutta methods is symplectic in their own right, and their \(b\)-values all have to agree.

**Proof.** Since \(I\) is a first integral, it holds that \(\sum_k B^k(y_k, f^k(y)) = 0\) for all \(y\). Specifically,
\[
\sum_{k} B^k(Y^i_k, F^i_k) = 0
\]
Inserting (7) into

\[ I(\tilde{y}) = \sum_{k} B^{k}(\tilde{y}_{k}, \tilde{y}_{k}) \]

we get

\[
I(\tilde{y}) = \sum_{k} B^{k} \left( y^{k} + h \sum_{i} b_{k}^{i} F_{i}^{k}, y^{k} + h \sum_{j} b_{j}^{k} F_{j}^{k} \right) \\
= I(y) + h \sum_{j} \sum_{k} b_{j}^{k} B^{k}(y^{j}, F_{j}^{k}) + h \sum_{i} \sum_{k} b_{i}^{k} B^{k}(F_{i}^{k}, y^{k}) \\
+ h^{2} \sum_{i,j} \sum_{k} b_{i}^{k} b_{j}^{k} B^{k}(F_{i}^{k}, F_{j}^{k})
\]

The trick now is to substitute \( y_{k} = Y_{i}^{k} - h \sum_{j} a_{i,j}^{k} F_{j}^{k} \) to get matching terms.

\[
I(\tilde{y}) = I(y) + h \sum_{i} \sum_{k} b_{i}^{k} B^{k}(Y_{i}^{k}, F_{i}^{k}) + h \sum_{i} \sum_{k} b_{i}^{k} B^{k}(F_{i}^{k}, Y_{i}^{k}) \\
+ h^{2} \sum_{i,j} \sum_{k} (b_{i}^{k} b_{j}^{k} - b_{j}^{k} a_{i,j}^{k} - b_{i}^{k} a_{i,j}^{k}) B^{k}(F_{i}^{k}, F_{j}^{k})
\]

We see that under the assumption \( b_{i}^{k} b_{j}^{k} - b_{j}^{k} a_{i,j}^{k} - b_{i}^{k} a_{i,j}^{k} = 0 \), the \( O(h^{2}) \) term disappears.

For the \( O(h) \) term, we see that if \( b_{i}^{k} = b_{i} \) is constant in \( k \), then

\[
2h \sum_{i} \sum_{k} b_{i}^{k} B^{k}(Y_{i}^{k}, F_{i}^{k}) = 2h \sum_{i} b_{i} = \sum_{k} B^{k}(Y_{i}^{k}, F_{i}^{k}) = 0,
\]

due to (8) \( \square \)

Now, let equation (6) be a Hamiltonian system given by \( H(y, z) \) of the form

\[
\frac{dy^{k}}{dt} = J^{-1}_{k} \frac{\partial H}{\partial y^{k}}
\]

where \( J_{k} \) are non-singular, skew-symmetric matrices.

Applying the above Theorem to the variational equation yields the following corollary

**Corollary 5.2.** If the coefficients satisfy that

(i) \( b_{i}^{k} b_{j}^{k} = b_{i}^{k} a_{i,j}^{k} + b_{j}^{k} a_{j,i}^{k} \) for all \( i, j, k \) and

(ii) \( b_{i}^{1} = b_{i}^{2} = \cdots = b_{i}^{N} \) for all \( i \).

Then the scheme is symplectic when applied to the system (9)

We now turn to the result actually needed in this paper, where each component is integrated with a partitioned Runge–Kutta method.
Consider a Hamiltonian system

\[
\begin{align*}
\frac{dq^k}{dt} &= \frac{\partial H}{\partial p^k} = f^k(q, p) \\
\frac{dp^k}{dt} &= -\frac{\partial H}{\partial q^k} = g^k(q, p) \quad k = 1, \ldots, N
\end{align*}
\]

We integrate the system with an integrator of the form

\[
\begin{align*}
\tilde{q}^k &= q^k + h \sum_{i=1}^s b^k_{ij} F^k_i \\
Q^k_i &= q^k + h \sum_{j=1}^s a^k_{ij} G^k_i \\
F^k_i &= f^k(Q^k_i, P^k_i) \\
P^k_i &= p^k + h \sum_{j=1}^s a^k_{ij} G^k_j \\
G^k_i &= g^k(Q^k_i, P^k_i)
\end{align*}
\]

**Theorem 5.3.** Assume we apply the scheme (7) to the Hamiltonian system (10). If the coefficients satisfy

(i) \( \hat{b}^k_j b^k_j = \hat{b}^k_j a^k_{ij} + b^k_j \hat{a}^k_{ji} \) for all \( i, j, k \),

(ii) \( b^k_i = \hat{b}^k_i \) for all \( k, i \) and

(iii) \( b^1_i = b^2_i = \cdots = b^N_i \) for all \( i \).

then the integrator is symplectic.

The proof of the theorem is analogous to the proof of 5.1, and is omitted.

6. Numerical experiments

Numerical tests were done on a simplified version of the spin-lattice-electron equations. In this system, the position and velocity of each particle is confined to a one-dimensional space. Furthermore, we use periodic boundaries in space and only consider forces between neighbouring particles.

The total Hamiltonian is

\[ H(w, q, p) = T_L(p) + U_L(q) + H_m(w, q) \]

where

\[ T_L(p) = \sum_{i=1}^N \frac{p_{i+1}^2}{2m_i} \]

\[ U_L(q) = \sum_{i=1}^n U(q_{i+1} - q_i) \]

\[ H_m(w, q) = \sum_{i=1}^n J(q_{i+1} - q_i) z_i^T z_{i+1} \]

To effectuate the periodic boundary, we define \( z_{N+1} = z_1 \) and \( q_{N+1} = q_1 + L \), where \( L \) is the period.
The intermolecular potential is the Lennart–Jones’ potential
\[ U(r) = U_0 \left[ \left( \frac{r_m}{r} \right)^{12} - 2 \left( \frac{r_m}{r} \right)^6 \right] \]
where \( r_m \) is the “rest distance” i.e. the distance at which \( U \) is minimal, and \( U_0 \) is a positive scalar which controls the strength of the interaction.

The magnetic force strength is a cubic function, of the same type as given by Ma, Woo and Dudarev [MWD08]
\[ J(r) = J_0 \cdot \left( 1 - \frac{r}{r_c} \right)^3 \cdot \Theta(r_c - r), \]
where \( \Theta \) is the Heaviside step function, and \( r_c \) is a cut-off distance. \( J_0 \) is a scalar which controls the strength of the magnetic interaction.

In the numerical tests performed, the values were set to,
\[ L = N = 30, \quad m_i = 1, \quad U_0 = 1, \quad r_m = 1, \quad J_0 = 10, \quad r_c = 1.5. \]

For initial data, we set
\[ q_k = k, \quad p_k = 0, \quad w_k = a_k \begin{bmatrix} 0.8 \cos \left( \frac{2\pi k}{n} \right) + 0.5 \sin \left( \frac{4\pi k}{n} \right) \\ 0.8 \sin \left( \frac{2\pi k}{n} \right) + 0.5 \cos \left( \frac{4\pi k}{n} \right) \\ 1 \end{bmatrix} \]
where \( a_k \) is chosen so that \( \| w_k \| = 1. \)

Figure 1 shows the long term behaviour of the energy terms \( T_L, U_L \) and \( H_m \) as well as their sum \( H \). (A constant term has been added to \( U_L \) to improve readability). The figure shows that while the energy is exchanged between the terms with an amplitude on the order of \( O(1) \), the variation in the sum is much smaller, on the order of \( O(10^{-3}) \).

The integrator was also tested with various stepsizes \( h \) from \( h = \frac{1}{16} \) down to \( h = 2^{-19} \) over the time interval \([0, 1]\) and the final values were compared with the
The same integrator using stepsize $h = 2^{-20}$. The resulting pseudoerrors are plotted in Figure 2. The plot shows the apparent second order of the integrator.

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