Symplectic integrators for classical spin systems

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Abstract

We suggest a numerical integration procedure for solving the equations of motion of certain classical spin systems which preserves the underlying symplectic structure of the phase space. Such symplectic integrators have been successfully utilized for other Hamiltonian systems, e. g. for molecular dynamics or non-linear wave equations. Our procedure rests on a decomposition of the spin Hamiltonian into a sum of two completely integrable Hamiltonians and on the corresponding Lie-Trotter decomposition of the time evolution operator. In order to make this method widely applicable we provide a large class of integrable spin systems whose time evolution consists of a sequence of rotations about fixed axes. We test the proposed symplectic integrator for small spin systems, including the model of a recently synthesized magnetic molecule, and compare the results for variants of different order.

Key words: symplectic integrators, classical spin systems
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1 Introduction

To calculate the time evolution of classical spin systems is an important task in condensed matter physics. For example, the cross section of neutron scattering at a spin system is proportional to the Fourier transform of the time-depending auto-correlation function, see [1], which can often be calculated in the classical limit. Completely integrable spin systems are rare, that is, in most cases an analytical calculation of the time evolution is not possible and one is lead

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to employ numerical integration methods. Since classical spin systems are instances of Hamiltonian systems, it is advisable to use numerical integrators which preserve the underlying symplectic structure of the phase space. Such "symplectic integrators" have been considered in the last decades [2] and have been applied to a variety of problems, ranging from molecular dynamics [3] to the nonlinear Schrödinger equation [4,5].
Unfortunately, symplectic integrators for spin systems have only rarely been considered in the literature, see [6,7,8]. The method of the independent time evolution of sublattices, proposed in [6,9,10], is volume-preserving but not symplectic, see 2.2.1 and [6]. Inspired by [10], we suggest to construct symplectic integrators based on a splitting of the spin Hamiltonian into two completely integrable Hamiltonians belonging to a special kind of systems [11,12]. These systems are called "$\mathcal{B}$-partitioned systems" and their time evolution can be calculated as a sequence of rotations about fixed axes [12]. This generalizes the Störmer/Verlet scheme based on separable Hamiltonians of the form $H = T(\mathbf{p}) + V(\mathbf{q})$.
In section 2 we provide the general definitions and results we need from analytical mechanics (section 2.1) and from the field of symplectic integrators based on Lie-Trotter decompositions of the time evolution operator (section 2.2). The reader who is not familiar with the differential geometric background may skip the technical details and only draw the moral that a symplectic integrator approximates the exact time evolution by a sequence of calculable time evolutions corresponding to auxiliary Hamiltonians. In section 3 we shortly recapitulate the theory of $\mathcal{B}$-partitioned systems from [12]. In order to test our suggestions we have implemented various variants of symplectic integrators and applied them to selected small spin systems, see section 4. We report the fluctuation of the total energy about its initial value as opposed to the constant drift for a non-symplectic Runge-Kutta method (RK4), see section 4.1. For two integrable spin systems we compare the errors of the various symplectic methods, including RK4, see sections 4.2.1 and 4.2.2. Finally, we compare the errors of five symplectic integrators for the integrable $N = 5$ spin pyramid and fixed runtime, see section 4.3. We close with a summary and outlook.

2 Definitions and general results

We will only formulate the pertinent definitions for symplectic integrators in the context of spin systems. For the general case there are excellent sources available in the literature, see e. g. [13,14] for analytical mechanics and [2] for symplectic integrators.

2.1 Generalities

Classical spin configurations can be represented by N-tuples of unit 3-vectors $\mathbf{s} = (\vec{s}_1, \ldots, \vec{s}_N)$, $|\vec{s}_\mu|^2 = 1$ for $\mu = 1, \ldots, N$. The compact, $2N$-dimensional manifold of all such configurations is the *phase space* of the spin system

$$\mathcal{P} = \mathcal{P}_N = \left\{ (\vec{s}_1, \ldots, \vec{s}_N) \,\middle|\, |\vec{s}_\mu|^2 = 1 \text{ for } \mu = 1, \ldots, N \right\} . \tag{1}$$

A special coordinate system is given by the $2N$ local functions φ_μ, $z_\mu : \mathcal{P} \to \mathbb{R}$, implicitly defined by

$$\vec{s}_\mu = \begin{pmatrix} \sqrt{1 - z_\mu^2} \cos \varphi_\mu \\ \sqrt{1 - z_\mu^2} \sin \varphi_\mu \\ z_\mu \end{pmatrix}, \ \mu = 1, \ldots, N . \tag{2}$$

A *tangent vector* of $\mathcal{P}$ at a point $\mathbf{s} \in \mathcal{P}$ can be represented by an N-tuple $\mathbf{t} = (\vec{t}_1, \ldots, \vec{t}_N)$ of 3-vectors satisfying the constraint

$$\vec{t}_\mu \cdot \vec{s}_\mu = 0, \ \mu = 1, \ldots, N . \tag{3}$$

If $\mathbf{a}, \mathbf{b}$ are two tangent vectors at $\mathbf{s} \in \mathcal{P}$, the assignment

$$\omega(\mathbf{a}, \mathbf{b}) = \sum_{\mu=1}^{N} (\vec{a}_\mu \times \vec{b}_\mu) \cdot \vec{s}_\mu \tag{4}$$

defines a non-degenerate, closed 2-form, that is, a *symplectic form* ω. In the coordinate system (2) ω can locally be written in the form

$$\omega = \sum_{\mu=1}^{N} d\varphi_\mu \wedge dz_\mu , \tag{5}$$

hence $(\varphi_\mu, z_\mu)_{\mu=1,\ldots,N}$ are canonical coordinates w. r. t. ω. The *volume form* $d\mathcal{P}$ is defined by

$$d\mathcal{P} = \omega^N = \omega \wedge \omega \wedge \ldots \wedge \omega \tag{6}$$

and has the local coordinate representation

$$d\mathcal{P} = d\varphi_1 \wedge dz_1 \wedge \ldots \wedge d\varphi_N \wedge dz_N . \tag{7}$$

A smooth Hamiltonian $H : \mathcal{P} \to \mathbb{R}$ generates the *Hamiltonian vector field* X_H implicitly defined by

$$i_{X_H}\, \omega \equiv \omega(X_H, \ ) = dH \ . \tag{8}$$

The corresponding Hamiltonian equations of motion are

$$\frac{d}{dt}\, \mathbf{s}(t) = X_H(\mathbf{s}(t)) \tag{9}$$

and assume their usual form

$$\frac{d}{dt}\varphi_\mu(t) = \frac{\partial H}{\partial z_\mu} \ , \qquad \frac{d}{dt} z_\mu(t) = -\frac{\partial H}{\partial \varphi_\mu} \ , \quad \mu = 1, \ldots, N \ , \tag{10}$$

in the canonical coordinate system (2). By writing the solution $\mathbf{s}(t)$ of (10) in the form $\mathbf{s}(t) = \mathcal{F}_t(H)(\mathbf{s}(0))$ we obtain the *Hamiltonian flow* $\mathcal{F}_t(H) : \mathcal{P} \to \mathcal{P}$. It is defined for all initial values $\mathbf{s}(0)$ and for all $t \in \mathbb{R}$ since $\mathcal{P}$ is compact, i. e. X_H is a *complete* vector field. Analogously, the flow of a general vector field can be defined.

A smooth map $\phi : \ \mathcal{P} \to \mathcal{P}$ is called *symplectic* iff it preserves the symplectic form, i. e. iff $\phi^*\omega = \omega$. Every symplectic map preserves the phase space volume, but not conversely, see the counter-example below. Any Hamiltonian flow $\mathcal{F}_t(H)$ is symplectic, cf. , for example, theorem 8.1.9 in [15]. Conversely, if the flow $\mathcal{F}_t$ of a complete vector field X is symplectic, then

$$\mathcal{L}_X \omega(\mathbf{s}) = \frac{d}{dt}\, \left(\mathcal{F}_t^* \omega\right)(\mathbf{s})\big|_{t=0} = 0 \ , \tag{11}$$

where $\mathcal{L}_X$ is the Lie derivative. Hence $0 = \mathcal{L}_X \omega = i_X\, d\omega + d i_X \omega = 0 + d i_X \omega$, that is, $i_X\omega$ is a closed 1-form, and has, by the Poincaré lemma, locally the form $i_X\omega = dK$. To summarize: symplectic flows are, at least locally, generated by suitable Hamiltonians K.

2.2 Symplectic integrators

From an abstract point of view, a *symplectic integrator* is an approximation of some exact flow $\mathcal{F}_t(H)$ by the composition of symplectic maps $\phi_\nu : \mathcal{P} \to \mathcal{P}$, which can be calculated analytically or numerically exact. In this article we

Table 1
Various decompositions of the form (16) which give rise to different symplectic integrators.

Name	Abbr.	Order	Coefficients	Ref.
Suzuki-Trotter	ST1	1	$a_1 = b_1 = \frac{1}{2}$	[16]
Suzuki-Trotter	ST2	2	$a_1 = a_2 = \frac{1}{2},\ b_1 = 1, b_2 = 0$	[17]
Suzuki-Trotter	ST4	4	$a_1 = a_6 = \frac{p}{2},\ b_6 = 0$ $b_1 = a_2 = b_2 = b_4 = a_5 = b_5 = p$ $a_3 = a_4 = \frac{1-3p}{2},\ b_3 = 1 - 4p$ $p = \frac{1}{4-4^{1/3}}$	[18]
Forest-Ruth	FR	4	$a_1 = a_4 = \frac{\theta}{2},\ a_2 = a_3 = \frac{1-\theta}{2}$ $b_1 = b_3 = \theta,\ b_4 = 0$ $b_2 = 1 - 2\theta,\ \theta = \frac{1}{2-2^{1/3}}$	[19]
Optimized Forest-Ruth	OFR	4	$a_1 = a_5 = \xi,\ a_2 = a_4 = \chi,\ b_5 = 0$ $a_3 = 1 - 2(\xi + \chi),\ b_1 = b_4 = \frac{1-2\lambda}{2}$ $b_2 = b_3 = \lambda = -0.09156203$ $\xi = 0.17208656,\ \chi = -0.16162176$	[20]

assume that the Hamiltonian H is decomposable into completely integrable Hamiltonians H_i in the form

$$H = \sum_i H_i \tag{12}$$

and that the ϕ_ν are the Hamiltonian flows corresponding to certain H_i. The precise form of the correspondence is given by a Lie-Trotter decomposition of the flow $\mathcal{F}_t(H)$ written as an exponential operator

$$\mathcal{F}_t(H) = e^{t\mathcal{H}} \ . \tag{13}$$

In order to make sense of (13) we have to linearize the Hamiltonian equations of motion. To this end we consider $\mathcal{F}_t(H)$ acting on functions $f : \mathcal{P} \to \mathbb{C}$ via

$$\mathcal{F}_t(H)^* f(\mathbf{s}) \equiv f\Big(\mathcal{F}_{-t}(H)(\mathbf{s})\Big) \ . \tag{14}$$

If f runs through $\mathcal{L}^2(\mathcal{P}, d\mathcal{P})$, the Hilbert space of (equivalence classes of) square-integrable complex functions, (14) defines a continuous, unitary 1-parameter group, see section 7.4 of [15] for details. By Stone's theorem, this

group has the form (13) with an anti-selfadjoint operator $\mathcal{H}$. One can show that $\mathcal{H}$ can be expressed by means of the Poisson bracket according to

$$\mathcal{H}f = \{H,\ f\} \equiv \omega(X_H, X_f), \qquad f \text{ smooth}\ , \tag{15}$$

but we will not need this in the sequel. (13) is only needed to provide a basis for using the techniques of Lie-Trotter decomposition for Hamiltonian flows.

For sake of simplicity let us consider the special case $H = H_1 + H_2$ and hence $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$. We are looking for ℓ-th order Lie-Trotter decompositions which have the form

$$e^{t(\mathcal{H}_1+\mathcal{H}_2)} = \prod_{i=1}^{k} e^{a_i t\mathcal{H}_1} e^{b_i t\mathcal{H}_2} + \mathcal{O}(t^{\ell+1})\ . \tag{16}$$

Both sides of (16) are expanded into power series in terms of t and set equal up to terms including t^ℓ. This yields a system of, in general, non-linear equations for the unknown coefficients $a_i,\ b_i$. Except for $\ell = 1$ the corresponding solutions are not unique. Hence there exist several decompositions and thus several symplectic integrators of the same order ℓ. In this article we will use the decompositions enumerated in table 1. All corresponding integrators are *symmetric*, or time-reversible, see [2]. Obviously, the Lie-Trotter decomposition (16) is a good approximation only for small t. Therefore the given time interval $[0, t]$ is usually split into L intervals of length Δ and (16) is separately applied to each time step Δ. Hence, apart from the choice of the decomposition, Δ is a further parameter of the integration procedure, see section 4.

2.2.1 A counter-example

It seems plausible that an arbitrary splitting $X_H = X_1 + X_2$ of a Hamiltonian vector field need not correspond to a splitting of the Hamiltonian $H = H_1 + H_2$, such that $X_i = X_{H_i}$ for $i = 1, 2$. Hence the decomposition $X_H = X_1 + X_2$ does not necessarily lead to symplectic integrators. Nevertheless, we will illustrate this by an example which is connected with a numerical integrator used for bi-partite spin systems, see [6,9,10]. Such spin systems can be divided into two disjoint subsets of spins A and B, such that the interaction is only non-zero between spins of different subsets. The first step of the numerical procedure consists of fixing the A-spins and calculating the time evolution of all B-spins. In the second step the role of A and B is interchanged, and so on. In a single step each spin of one subset rotates about the fixed (weighted) sum of all its neighboring spins; hence the numerical integrator preserves the volume of the total phase space. But, as we will show, this integrator is not symplectic, see

also the corresponding remark in [6].
It suffices to consider just two spins and a single step of the described numerical integrator which solves the equations of motion

$$\frac{d}{dt}\vec{s}_1 = \vec{s}_2 \times \vec{s}_1, \quad \frac{d}{dt}\vec{s}_2 = \vec{0}\,, \tag{17}$$

defining a vector field X on $\mathcal{P}_2$. We adopt canonical coordinates $\varphi_1, z_1, \varphi_2, z_2$ defined in (2) and use the local expression $\omega = d\varphi_1 \wedge dz_1 + d\varphi_2 \wedge dz_2$ of the symplectic form. After some elementary calculations we obtain

$$\begin{aligned} i_X\omega &= \dot{\varphi}_1 dz_1 - \dot{z}_1 d\varphi_1 && (18)\\ &= \left(z_2 - z_1\sqrt{\tfrac{1-z_2^2}{1-z_1^2}}\cos(\varphi_1-\varphi_2)\right) dz_1 \\ &\quad -\sqrt{(1-z_1^2)(1-z_2^2)}\sin(\varphi_1-\varphi_2)d\varphi_1\,. && (19)\end{aligned}$$

Obviously, $i_X\omega$ is not closed, and hence X does not generate a symplectic flow, cf. the discussion after (11).

3 $\mathcal{B}$-partitioned spin systems

The symplectic integrators considered in section 2.2 are based on a splitting of the spin Hamiltonian into a sum of completely integrable Hamiltonians: $H = \sum_i H_i$. For Heisenberg Hamiltonians

$$H(\mathbf{s}) = \sum_{\mu<\nu} J_{\mu\nu}\vec{s}_\mu \cdot \vec{s}_\nu\,, \qquad \text{where } J_{\mu\nu} \in \mathbb{R}\,, \tag{20}$$

such a splitting is always possible; in fact, each summand in (20) is a completely integrable dimer Hamiltonian. However, it seems favorable to work with as few summands as possible, or, equivalently, to work with "large" integrable Hamiltonians. To this end we will define a special class of completely integrable spin systems called $\mathcal{B}$-partitioned systems, following [12].
As an example, consider the Heisenberg Hamiltonian of the spin square

$$H_\square = \vec{s}_1 \cdot \vec{s}_2 + \vec{s}_2 \cdot \vec{s}_3 + \vec{s}_3 \cdot \vec{s}_4 + \vec{s}_4 \cdot \vec{s}_1\,. \tag{21}$$

It is integrable because it can be written as

$$H_\square = \tfrac{1}{2}\left((\vec{s}_1+\vec{s}_2+\vec{s}_3+\vec{s}_4)^2 - (\vec{s}_1+\vec{s}_3)^2 - (\vec{s}_2+\vec{s}_4)^2\right)\,. \tag{22}$$

The grouping of the spins in (22) can be encoded in a "partition tree"

$$\mathcal{B}_{\square} = \{\{1,2,3,4\},\{1,3\},\{2,4\},\{1\},\{2\},\{3\}\,\{4\}\}\,. \tag{23}$$

Generalizing this example, we define

Definition 1 *A partition tree $\mathcal{B}$ over a finite set $\{1,\ldots,N\}$ is a set of subsets of $\{1,\ldots,N\}$ satisfying*

(1) $\emptyset \notin \mathcal{B}$ and $\{1,\ldots,N\} \in \mathcal{B}$,
(2) for all $M, M' \in \mathcal{B}$ either $M \cap M' = \emptyset$ or $M \subset M'$ or $M' \subset M$,
(3) for all $M \in \mathcal{B}$ with $|M| > 1$ there exist $M_1, M_2 \in \mathcal{B}$ such that $M = M_1 \dot{\cup} M_2$.

It follows from definition 1 (2) that the subsets M_1, M_2 satisfying $M = M_1 \dot{\cup} M_2$ in definition 1 (3) are unique, up to their order. M_1, M_2 are hence defined for all $M \in \mathcal{B}$ with $|M| > 1$. M_1 and M_2 denote the two uniquely determined "branches" starting from M. It follows that $\mathcal{B}$ is a binary tree with the root $\{1,\ldots,N\}$ and singletons $\{\mu\}$ as leaves. More general partitions into k disjoint subsets can be reduced to subsequent binary partitions and hence need not be considered. For all $M \in \mathcal{B}$ there is a unique path

$$\mathcal{P}_M(\mathcal{B}) \equiv \{M' \in \mathcal{B} \mid M \subset M'\} \tag{24}$$

joining M with the root of $\mathcal{B}$. It is linearly ordered since $M \subset M'$ and $M \subset M''$ imply $M' \subset M''$ or $M'' \subset M'$ by definition 1 (2). Especially, every element $\mu \in \{1,\ldots,N\}$ belongs to a unique, linearly ordered *construction path*

$$\mathcal{P}_\mu(\mathcal{B}) \equiv \{M \in \mathcal{B} \mid \mu \in M\}\,. \tag{25}$$

For $\mu \neq \nu \in \{1,\ldots,N\}$ let $M_{\mu\nu} \in \mathcal{B}$ denote the smallest set of $\mathcal{B}$ such that $\mu, \nu \in M_{\mu\nu}$, i. e. $M_{\mu\nu} \in \mathcal{B}$ is the set where both construction paths of μ and ν meet the first time. For $M \neq \{1,\ldots,N\}$ we will denote by $\overline{M}$ the "successor" of M, that is, the smallest element of $\mathcal{P}_M(\mathcal{B})$ except M itself.

Consider real functions J defined on a partition tree

$$J : \mathcal{B} \longrightarrow \mathbb{R} \tag{26}$$

satisfying $J(\{\mu\}) = 0$ for all $\mu = 1,\ldots,N$. Then

$$H = \sum_{\mu<\nu} J(M_{\mu\nu})\vec{s}_\mu \cdot \vec{s}_\nu \tag{27}$$

defines a Heisenberg Hamiltonian. The corresponding spin system will be called a $\mathcal{B}$-*partitioned system* or sometimes, more precisely, a $(\mathcal{B}, J)-$*system*. For example, the spin square (21) is obtained by the partition tree (23) and by the function J with $J(\{1,2,3,4\}) = 1$ and $J(M) = 0$ else.

Let $\vec{S}_M$ denote the total spin vector of the subsystem $M \subset \{1,\ldots,N\}$ with length S_M. Further, let $\mathbb{D}(\vec{\omega}, t)$ denote the 3-dimensional rotation matrix with axis $\vec{\omega}$ and angle $|\vec{\omega}|\, t$. In the special case $\vec{\omega} = \vec{0}$, $\mathbb{D}(\vec{\omega}, t)$ denotes the identity matrix $\mathbb{I}$. Then the following can be proven, see [12]:

Theorem 2 *Let H be the Hamiltonian of a $(\mathcal{B}, J)$-system. Then its time evolution is given by*

$$\vec{s}_\mu(t) = \overleftarrow{\prod}_{M \in \mathcal{P}_\mu(\mathcal{B})} \mathbb{D}\left(\vec{S}_M(0), (J(M) - J(\overline{M}))t\right) \quad \vec{s}_\mu(0)\ , \quad \mu = 1,\ldots,N, \quad (28)$$

where the arrow above the product symbol denotes a product according to a decreasing sequence of sets $M \in \mathcal{P}_\mu(\mathcal{B})$ from left to right and $J(\overline{M}) \equiv 0$ for $M = \{1,\ldots,N\}$.

We note that the time evolution in the presence of a Zeeman term in a Hamiltonian of the form $H + \vec{B} \cdot \vec{S}$, where $\vec{B}$ is the dimensionless magnetic field, is obtained by multiplying (28) from the left with $\mathbb{D}(\vec{B}, t)$.

If we stick to the symplectic integrators of table 1 and to $\mathcal{B}$-partitioned systems as completely integrable spin systems, our method only applies to those spin systems whose Hamiltonian can be written as the sum of two Hamiltonians of $\mathcal{B}$-partitioned subsystems. The spin cube with one additional space diagonal is an example which can only be decomposed into at least three $\mathcal{B}$-partitioned subsystems. But our method can, in principle, be extended to decompositions of the Hamiltonian into more than two summands. As an non-trivial example where our method works without modification we mention the spin system of $N = 30$ spins which are uniformly coupled according to the edges of an icosidodecahedron, see [21]. Such a spin system has been physically realized as an organic molecule containing 30 paramagnetic Fe-ions, see [22]. In figure 1 the planar graph of the icosidodecahedron is decomposed into two $\mathcal{B}$-partitioned subsystems A and B. A consists of 6 disjoint "bow ties" of the form $\bowtie$ and B of 8 disjoint triangles together with 6 single spins.

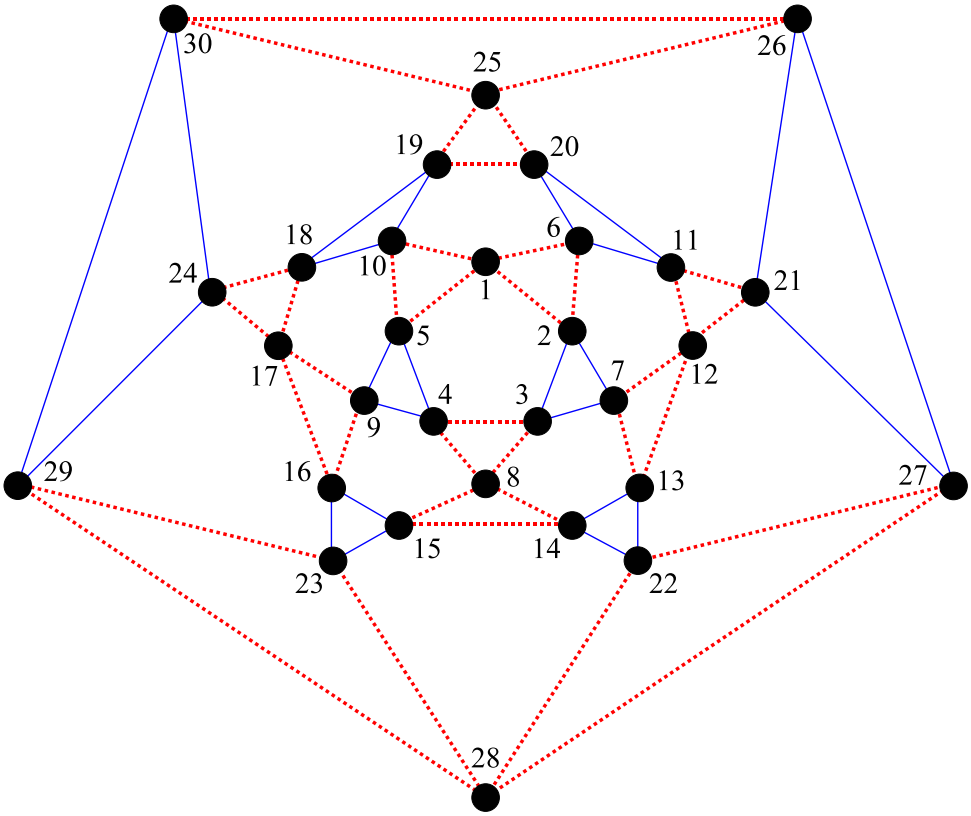

Fig. 1. Decomposition of the graph of the icosidodecahedron into 6 bow ties (dashed lines) and 8 triangles (solid lines). This is the basis of the symplectic integrators approximately solving the equations of motion for the corresponding classical spin system.

4 Results

We have implemented the various symplectic integrators described above using the computer algebra software MATHEMATICA 4.0 and have applied them to small spin systems. This seems to be sufficient in order to test general properties of the algorithms and to compare the different decompositions according to table 1. For more extensive tests and "real life" applications an implementation using other computer languages would be advisable.
For a non-integrable spin system it is impossible to compare the results of a numerical integration with the exact result since the exact result is not known by definition. Possible tests are observations of conserved quantities as the total energy H for non-integrable spin systems or observations of non-conserved quantities for integrable spin systems. These tests will be reported and discussed in the next subsections.

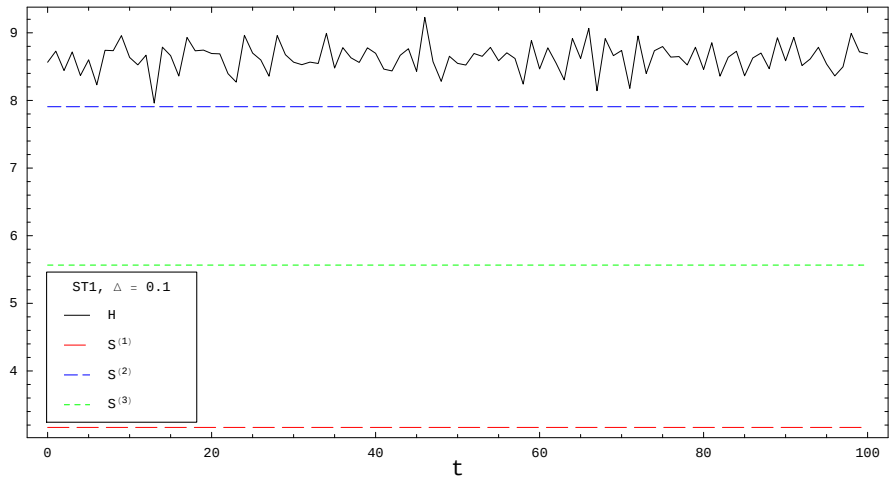

Fig. 2. Total energy and the three components of the total spin $\vec{S}$ of the icosidodecahedron as a function of time calculated by ST1.

4.1 Total energy

Figure 2 and 3 show results of numerical integrations of the Hamiltonian equations of motion for the spin system corresponding to the icosidodecahedron, see figure 1. We choose physical units such that the coupling constant J assumes the value 1. For all integrations the time interval is chosen as $[0, 100]$ and the time step is $\Delta = 0.1$. The initial spin configuration is chosen randomly. The symplectic integrators applied to this problem are based on a decomposition of the icosidodecahedron into 6 bow ties and 8 triangles as explained above.
Figure 2 shows the total energy and the three components of the total spin $\vec{S}$ as a function of time calculated by the first order integrator ST1. Whereas $\vec{S}$ is exactly conserved by all symplectic integrators considered in this article, the total energy fluctuates about its initial value with a maximal deviation of approximately 7%.
For symplectic integrators of 4th order the same behavior of the total energy can be observed, except that the range of the fluctuation is much smaller. The absolute maximal deviation is about $5 \cdot 10^{-4}$ for FR and $5 \cdot 10^{-5}$ for OFR and ST4, see figure 3. In contrast to these results, a 4th order Runge-Kutta method (RK4) yields a systematic drift of the total energy which reaches a deviation of $1.5 \cdot 10^{-3}$ at $t = 100$. This is typical for non-symplectic integrators, see [2], and one of the main reasons to adopt symplectic methods for Hamiltonian systems.

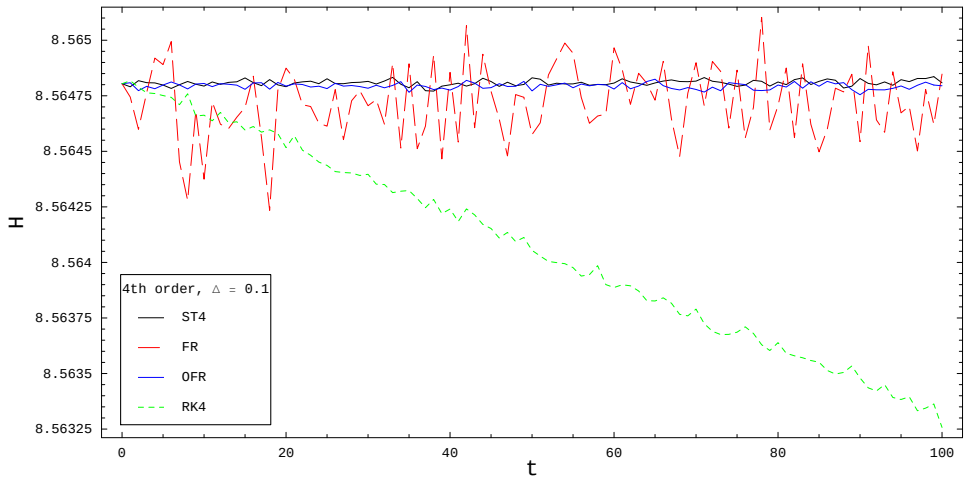

Fig. 3. Total energy of the icosidodecahedron as a function of time calculated by ST4, FR, OFR and RK4.

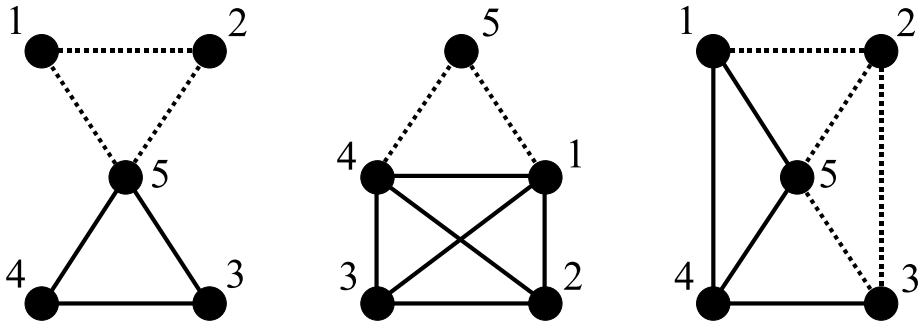

Fig. 4. Three integrable spin systems used for tests of numerical integrators: The bow tie, Nicholas' house and the pyramid. The decomposition into integrable subsystems used for symplectic integrators is indicated by solid and dashed lines.

4.2 Comparison with exact solutions

We compare non-conserved quantities calculated by the various numerical methods with the exact solutions for two integrable systems, the bow tie and "Nicholas' house", see figure 4. The latter is named after a German nursery-rhyme ("Das ist das Haus vom Nikolaus"). The time interval $[0, 100]$, the time step $\Delta = 0.1$ and the random choice of the initial configuration is similar as in the previous sections. Although the results of the comparison with exact solutions shed some light on the respective merits of the different methods, it seems dangerous to generalize them to non-integrable problems where the distance between near-by solutions may increase exponentially.

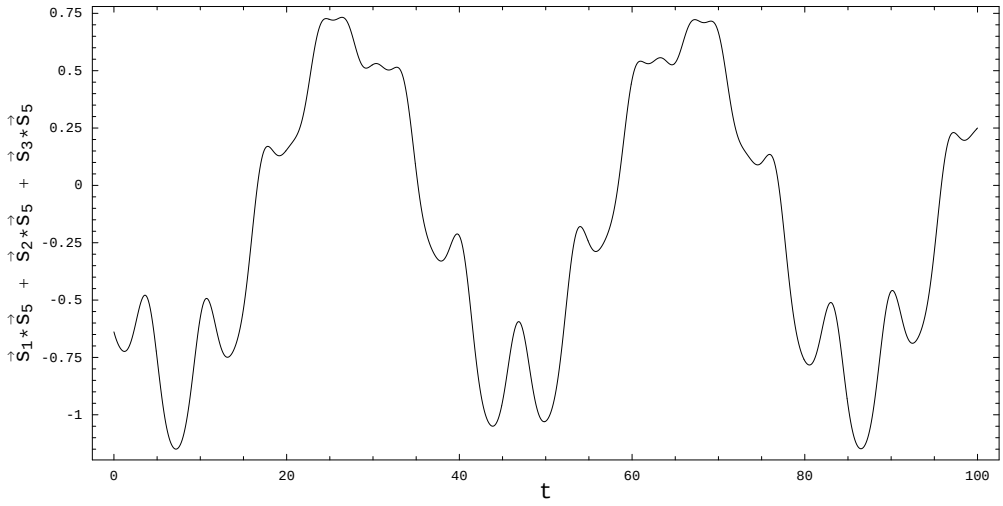

Fig. 5. $\vec{s}_1 \cdot \vec{s}_5 + \vec{s}_2 \cdot \vec{s}_5 + \vec{s}_3 \cdot \vec{s}_5$ as an exact function of time for the bow tie.

4.2.1 Bow tie

Figure 5 shows the quantity $\vec{s}_1 \cdot \vec{s}_5 + \vec{s}_2 \cdot \vec{s}_5 + \vec{s}_3 \cdot \vec{s}_5$ as an exact function of time. Figure 6 shows the absolute deviation $\delta(\vec{s}_1 \cdot \vec{s}_5 + \vec{s}_2 \cdot \vec{s}_5 + \vec{s}_3 \cdot \vec{s}_5)$ between the numerical and the exact value in logarithmic scale for the 4th order integrators considered above. These deviations seem to increase linearly in time (note the logarithmic scale) but with different orders of magnitude. The sharp minima of the logarithmic deviations in this and the following figures are due to intersections between the exact and the approximate functions. At $t = 100$ the four integrators can be ordered into a decreasing sequence according to their deviations, namely FR, RK4, OFR, ST4, where the ratio between two neighbors of this sequence is approximately a factor of 10. It is somewhat surprising that the non-symplectic RK4 is better than FR, but w r. t. conserved quantities FR should outperform RK4, as shown in section 4.1.

4.2.2 Nicholas' house

It is advisable to consider another example in order to see whether the above findings for the bow tie are typical. Figure 7 shows the quantity $\vec{s}_1 \cdot \vec{s}_3 + \vec{s}_2 \cdot \vec{s}_4$ for the spin system called "Nicholas' house" as an exact function of time. Figure 8 shows the absolute deviation $\delta(\vec{s}_1 \cdot \vec{s}_3 + \vec{s}_2 \cdot \vec{s}_4)$ between the numerical and the exact value in logarithmic scale for the 4th order integrators considered above. These deviations seem to increase again linearly in time (note the logarithmic scale). At $t = 100$ we have two groups, (FR, RK4) and (OFR, ST4) with comparable deviations within these groups, where the deviations of the second group are almost two orders of magnitude smaller that those of the first group.

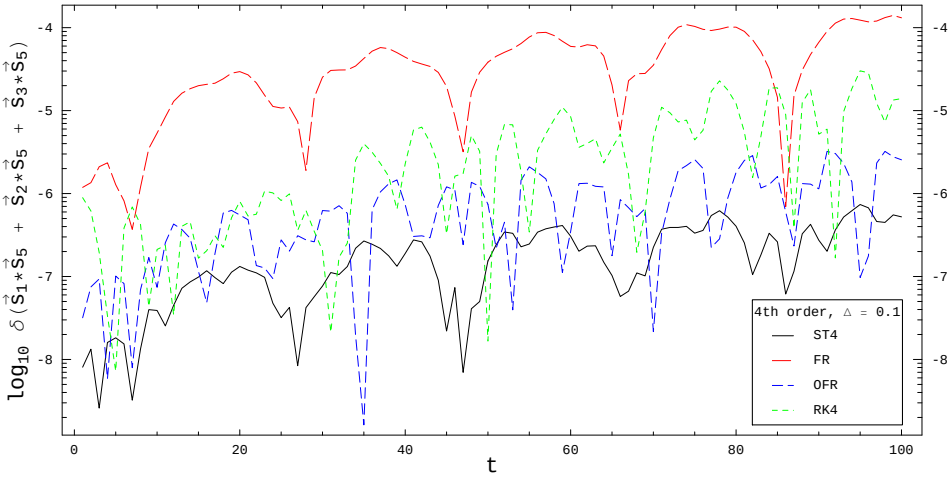

Fig. 6. $\log_{10}\delta(\vec{s}_1\cdot\vec{s}_5+\vec{s}_2\cdot\vec{s}_5+\vec{s}_3\cdot\vec{s}_5)$ as a function of time for the bow tie and the integrators ST4, FR, OFR, and RK4.

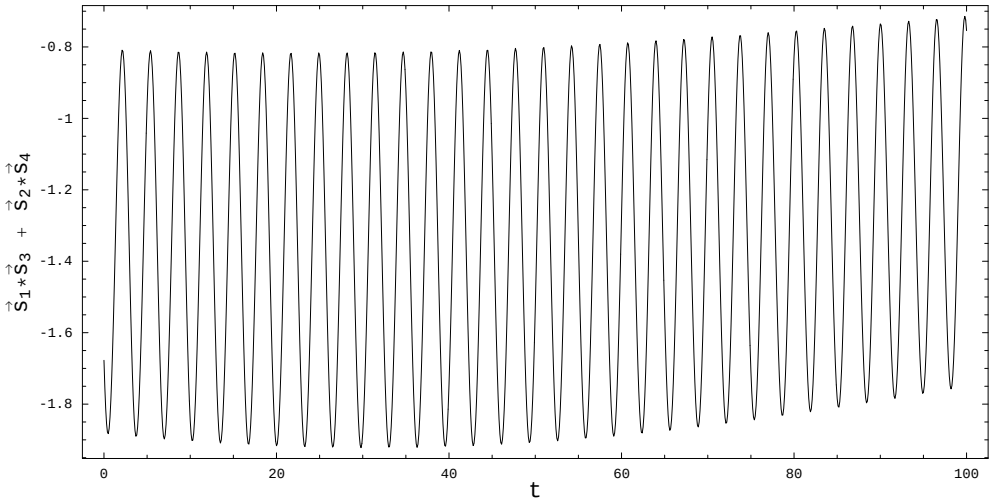

Fig. 7. $\vec{s}_1\cdot\vec{s}_3+\vec{s}_2\cdot\vec{s}_4$ as an exact function of time for Nicholas' house.

4.3 Comparison for given runtime

From a practical point of view it is not important which numerical procedure shows the smallest deviations for a fixed time step Δ but rather for a fixed runtime. We will provide a first test of this kind. For this test we have to exclude the Runge-Kutta procedures since they are implemented in the NDSolve-command of MATHEMATICA and hence their runtime cannot be compared with the symplectic integrators programmed in MATHEMATICA code. The NDSolve-command of MATHEMATICA 5.0 also allows the choice of symplectic integrators, but these integrators are not suited for spin systems since they rest on a splitting of the form $H = T(\mathbf{p}) + V(\mathbf{q})$, where $\mathbf{p}, \mathbf{q}$ are

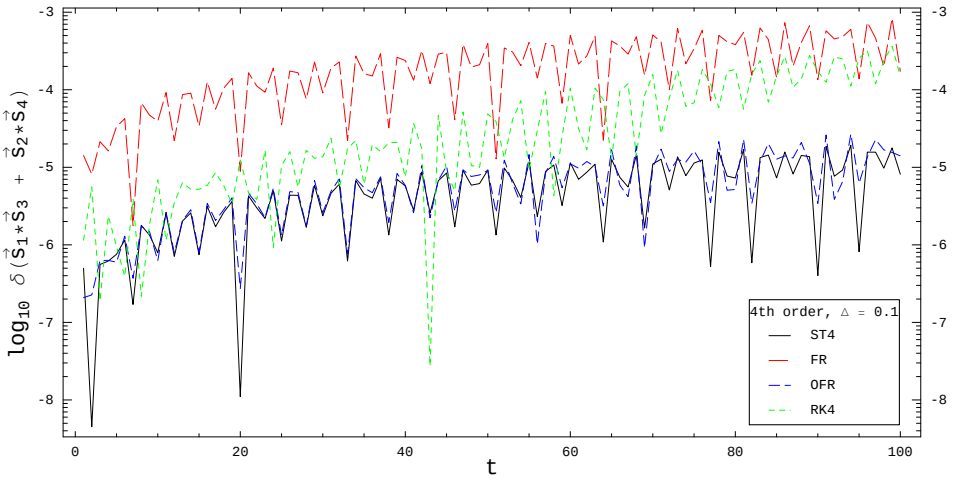

Fig. 8. $\log_{10}\delta(\vec{s}_1\cdot\vec{s}_3+\vec{s}_2\cdot\vec{s}_4)$ as a function of time for Nicholas' house and the integrators ST4, FR, OFR, and RK4.

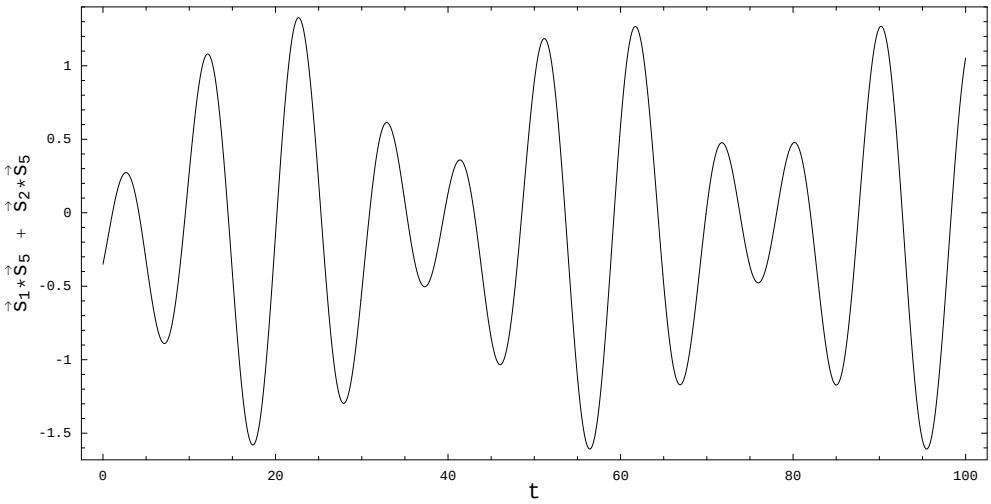

Fig. 9. $\vec{s}_1\cdot\vec{s}_5+\vec{s}_2\cdot\vec{s}_5$ as an exact function of time for the pyramid.

sets of canonical coordinates.

The runtime will be measured in terms of the number of "basic operations". A basic operation is the calculation of the exact time evolution $\mathcal{F}_\Delta(H_i)$ for the Hamiltonian H_i of an integrable subsystem. All basic operations approximately require the same cpu-time. The common task is to calculate the quantity $\vec{s}_1\cdot\vec{s}_5+\vec{s}_2\cdot\vec{s}_5$ as a function of $t\in[0,100]$ for a random start configuration of the spin pyramid, see figure 4, using maximal 10.000 basic operations. For every numerical procedure the appropriate step size Δ is separately chosen. The results are compared with the exact solution, see figure 9, and the deviations are plotted as functions of t in logarithmic scale, see figure 10. The deviations

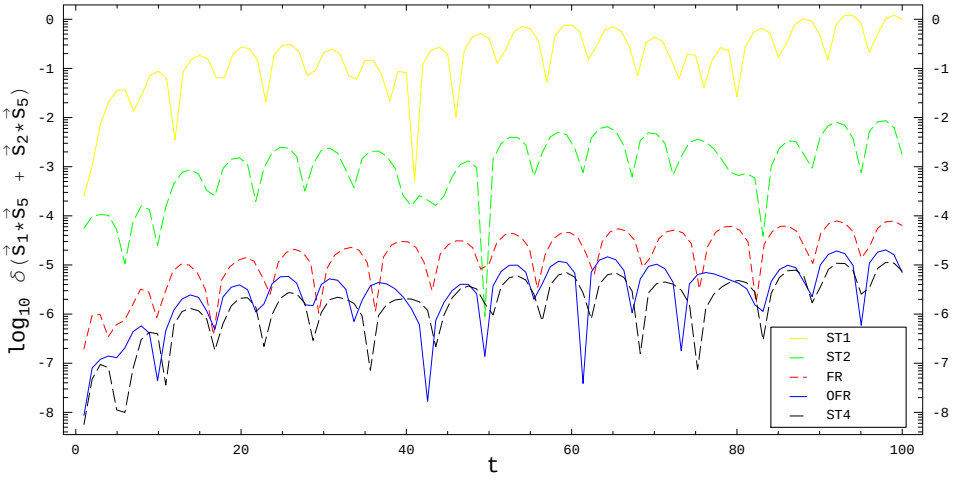

Fig. 10. $\log_{10} \delta(\vec{s}_1 \cdot \vec{s}_5 + \vec{s}_2 \cdot \vec{s}_5)$ as a function of time for the pyramid and the integrators ST1, ST2, ST4, FR, and OFR.

vary over 8 orders of magnitude and seem to increase with t. It turns out that ST4 is three orders of magnitude more precise than ST2 and even five orders of magnitude more precise than ST1. Whereas FR lies between ST2 and ST4, OFR is close to ST4, although its maximal deviation is about two times larger than that of ST4. These results indicate that it might be worth while to adopt symplectic integrators of even higher order, say, for example, ST6 or ST8.

5 Summary and outlook

We have proposed a symplectic integrator scheme for classical spin systems based on a splitting of the spin Hamiltonian into two completely integrable components corresponding to $\mathcal{B}$-partitioned subsystems. Further, we have implemented several variants of this integrator for a selection of small spin systems and performed certain tests and comparisons. The results largely conform with the expectations; an interesting finding is that, for fixed runtime, higher order algorithms yield marked improvements of the precision. This accords with the results of [2], section V.3.2, where, however, no further improvement occurs beyond the order of 8.
Of course, these tests are only preliminary and should be extended to include, for instance, more spin systems, the longtime behavior and the influence of different decompositions of the Hamiltonian. Also we have not compared our method with other methods which are energy- and volume-preserving, but not symplectic [6,9,10]. Our method cannot be applied to an arbitrary Hamiltonian spin system without taking additional measures. This is a draw-back, but simultaneously an advantage since it means that one has to adapt the method for a given system in order to find an optimal algorithm. In view of the ap-

plicability the perhaps most pressing generalization would be to consider the case of more than two integrable components of the Hamiltonian.

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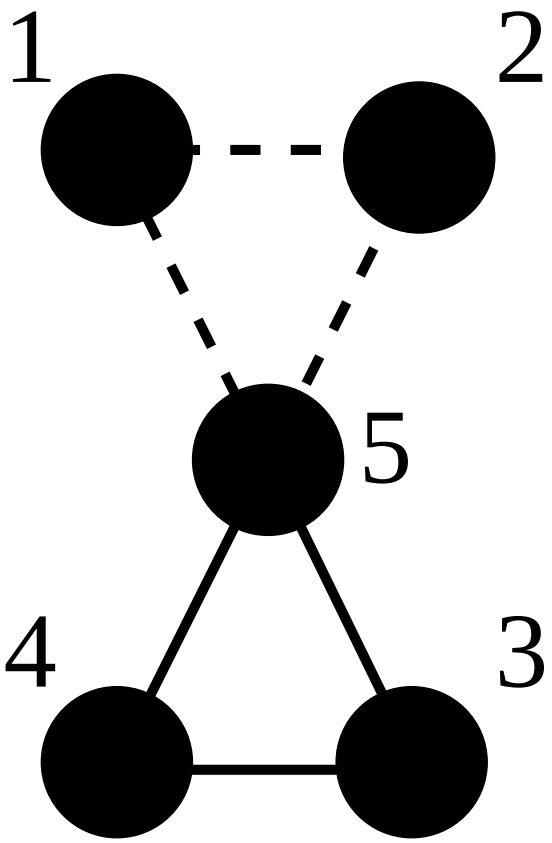
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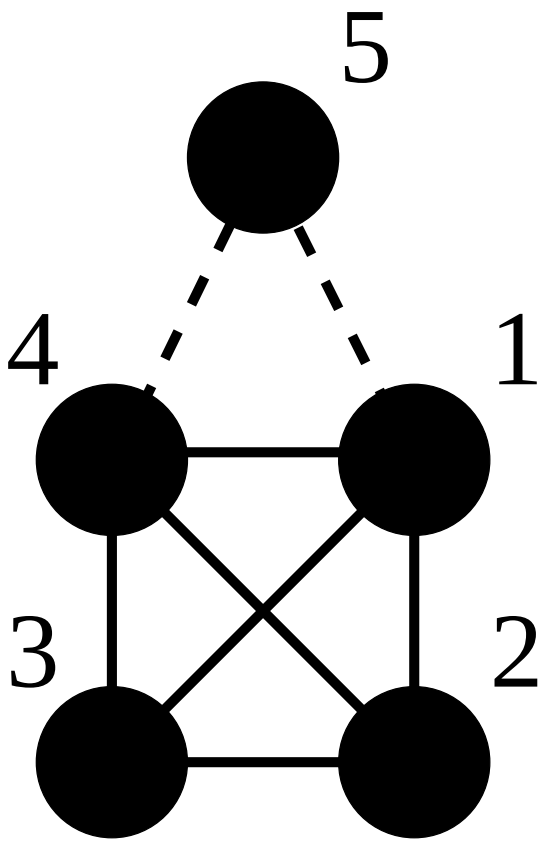
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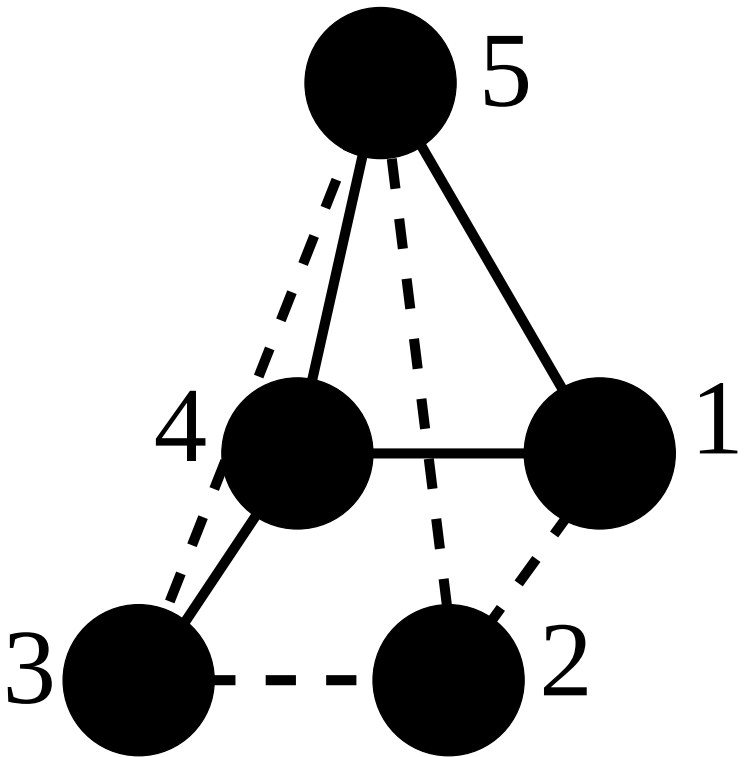
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