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SYMPLECTIC METHODS BASED ON DECOMPOSITIONS*

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Abstract. We consider methods that integrate systems of differential equations $dy/dt = f(y)$ by taking advantage of a decomposition of the right-hand side $f = \sum f^{[\nu]}$. We derive a general necessary and sufficient condition for those methods to be symplectic for Hamiltonian problems. Special attention is given to the case of additive Runge–Kutta methods.

Key words. additive Runge–Kutta method, symplectic integration, splitting

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1. Introduction. The purpose of this paper is to provide a necessary and sufficient condition for the symplecticness of numerical methods based on decompositions of the right-hand side of the system of differential equations being integrated.

Most numerical methods [4], [12] for the integration of systems of differential equations

$$\frac{dy}{dt} = f(y) \tag{1}$$

use the right-hand side f only through a subroutine that finds $f(y)$ at any given point y. Other methods require, in addition, subroutines for the evaluation of the Jacobian $f'(y)$ or of higher derivatives of f. All these methods, by ignoring all details of the structure of f, may provide general-purpose, black-box library integrators. However, in many applications, f possesses, in a natural way, a decomposition

$$f(y) = \sum_{\nu=1}^{N} f^{[\nu]}(y), \tag{2}$$

and one may wish to consider methods that take advantage of the structure of f. Those methods, while not very well suited to the construction of general-purpose integrators, can be useful for large problems arising in specific applications.

Splitting methods provide an obvious example: if the systems

$$\frac{dy}{dt} = f^{[\nu]}(y), \qquad \nu = 1, \dots, N, \tag{3}$$

are integrable in closed form, it is possible to integrate (1) by combining individual solutions of (3). If the systems (3), without being integrable in closed form, are "simpler" than (1), it is possible to combine numerical approximations to the solutions

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of (3) to obtain a numerical solution to (1). Splitting methods are often used in time-dependent partial differential equations; the different $f^{[\nu]}$ may correspond to different spatial variables (dimensional splitting) or to different physical contributions, e.g., advection and diffusion (operator splitting). The literature on splitting methods is, of course, huge, and we cannot review it here; we nevertheless mention the important recent paper [16].

If, in (2), $N = 2$ and $f^{[1]}$ is stiff while $f^{[2]}$ is not, then it is common to combine an implicit integrator for $f^{[1]}$ with an explicit integrator for $f^{[2]}$. For instance, in a reaction-diffusion partial differential problem, one may combine the implicit midpoint rule for the diffusion terms with the second-order Adams–Bashforth for the reaction terms. An interesting recent paper in this direction is [2]. Cooper and Sayfy [7], [8] have considered general classes of such *additive* methods, including (N-part) additive Runge–Kutta (ARK$_N$) methods. A step $y_n \mapsto y_{n+1}$ of the s-stage ARK$_N$ method specified by the Butcher tableau

$$\begin{array}{|ccc|c|ccc}
a_{11}^{[1]} & \cdots & a_{1s}^{[1]} & & a_{11}^{[N]} & \cdots & a_{1s}^{[N]} \\
\vdots & \ddots & \vdots & \cdots & \vdots & \ddots & \vdots \\
a_{s1}^{[1]} & \cdots & a_{ss}^{[1]} & & a_{s1}^{[N]} & \cdots & a_{ss}^{[N]} \\
\hline
b_1^{[1]} & \cdots & b_s^{[1]} & \cdots & b_1^{[N]} & \cdots & b_s^{[N]}
\end{array} \tag{4}$$

is given by

$$Y_{n,i} = y_n + h \sum_{\nu=1}^{N} \sum_{j=1}^{s} a_{ij}^{[\nu]} f^{[\nu]}(Y_{n,j}), \tag{5}$$

$$y_{n+1} = y_n + h \sum_{\nu=1}^{N} \sum_{i=1}^{s} b_i^{[\nu]} f^{[\nu]}(Y_{n,i}). \tag{6}$$

When the $a_{ij}^{[\nu]}$, $b_i^{[\nu]}$ do not depend on ν the ARK$_N$ method applied to the decomposed system (1)–(2) is equivalent to a standard Runge–Kutta method applied to the undecomposed (1). ARK$_N$ methods have recently been considered in Jorge's thesis [14].

In molecular dynamics applications the different $f^{[\nu]}$ may correspond to forces of different stiffness. It is sometimes inappropriate to sample the net force f; one may wish to sample the stiffer parts $f^{[\nu]}$ more frequently than the softer parts. This leads to the idea of *multiple time-step methods*; see, e.g., [3].

Another decomposition that often appears in practice is that provided by *component partitioning*, as in Hairer [9]: the set of the indices i that number the solution components y^i is partitioned into N subsets $\mathcal{I}^{[\nu]}$ and

$$f^{[\nu]i}(y) = \begin{cases} f^i(y), & i \in \mathcal{I}^{[\nu]}, \\ 0, & i \notin \mathcal{I}^{[\nu]}. \end{cases} \tag{7}$$

Coordinate partitioning arises naturally if (1) has been obtained by rewriting as a first-order system a system $y^{(N)} = F(y, \ldots, y^{(N-1)})$ of order N; in this case the blocks $\{y^i : i \in \mathcal{I}^{[\nu]}\}$ correspond to the time-derivatives $y^{(\nu)}$ of the solution y. Hamiltonian systems have their solution components partitioned in a natural way into coordinates and momenta. In some stiff problems some components are not stiff and one may wish to treat them separately; this leads to partitioning in stiff and nonstiff components.

In this paper we consider the case where (1) is a Hamiltonian system. We are interested in methods based on decompositions (2) that are symplectic [20], [22], [12].

If the parts $f^{[\nu]}$ *are themselves Hamiltonian,* then it is easy to construct symplectic NB-series methods by concatenating symplectic methods applied to the individual parts of the right-hand side or to linear combinations of those individual parts. As a first example with $N = 2$, we have the splitting methods of the form [16]

$$\phi_{\beta_s h, f^{[2]}} \circ \phi_{\alpha_s h, f^{[1]}} \circ \cdots \circ \phi_{\beta_2 h, f^{[2]}} \circ \phi_{\alpha_2 h, f^{[1]}} \circ \phi_{\beta_2 h, f^{[2]}} \circ \phi_{\alpha_1 h, f^{[1]}}. \tag{8}$$

Here α_i and β_i are real constants and $\phi_{h,g}$ denotes the exact solution flow of the system with right-hand side g. A second example, also with $N = 2$, is given by the time-symmetric concatenation

$$\psi^{\mathrm{MP}}_{h,\alpha f^{[1]}} \circ \psi^{\mathrm{MP}}_{h,(1-2\alpha) f^{[1]} + f^{[2]}} \circ \psi^{\mathrm{MP}}_{h,\alpha f^{[1]}}, \tag{9}$$

where α is a real constant and $\psi^{\mathrm{MP}}_{h,g}$ denotes a step of length h of the implicit midpoint rule applied to the system with right-hand side g. Clearly, (9) is a multiple time-step method that uses $f^{[2]}$ less frequently than $f^{[1]}$; it is also the ARK_2 method with tableau

$$\begin{array}{|ccc|ccc}
\frac{\alpha}{2} & 0 & 0 & 0 & 0 & 0 \\
\alpha & \frac{1-2\alpha}{2} & 0 & 0 & \frac{1}{2} & 0 \\
\alpha & 1-2\alpha & \frac{\alpha}{2} & 0 & 1 & 0 \\
\hline
\alpha & 1-2\alpha & \alpha & 0 & 1 & 0
\end{array}\,. \tag{10}$$

It is worth noting that the multiple time-stepping algorithms used in practice can similarly be reformulated as ARK methods. By concatenating steps of (9) as in [22, Section 13.1] it is possible to obtain symplectic ARK methods of arbitrarily high orders.

It is then of interest to characterize those decomposition methods that are symplectic. To provide a treatment as comprehensive as possible, we note that any reasonable one-step method based on the decomposition (2) gives rise, by Taylor-expanding the numerical solution in powers of the step-size h, to a so-called NB-series [14]. It is then convenient to work at the level of NB-series, rather than at the level of specific classes of methods, and in section 3 we provide necessary and sufficient conditions for a transformation given as an NB-series to be symplectic. Two scenarios are considered. In the first, the individual parts $f^{[\nu]}$ are supposed to be Hamiltonian. As discussed above, there are then symplectic decomposition methods, and the characterization in section 3.1 can be used either *positively* to construct new symplectic methods or *negatively* to show that symplectic integrators with some target properties are not possible. In the second scenario, the arbitrary (Hamiltonian) problem (1) is arbitrarily decomposed into N *not necessarily Hamiltonian* parts. We then prove that there is no genuine symplectic NB-series, in the sense that any symplectic NB-series uses only the net right-hand side f, rather than the individual parts $f^{[\nu]}$.

It is by now well understood [22], [12] that for symplectic methods some of the standard order conditions become redundant. In section 4 we study the reduction of independent order conditions for symplectic NB-series methods.

Section 5 deals with the situation where $N = 2$ and the decomposition has been carried out by partitioning the components into coordinates and momenta. We emphasize that, due to the extra structure implied by component partitioning, the material in this section is not just the particular case $N = 2$ of the theory presented in sections 3 and 4. Sections 3–5 provide a unified theory of symplectic methods and their order conditions that includes all cases known at present.

In section 6 we consider ARK_N methods. For this class of methods, the general symplecticness condition of section 3 may be rewritten in terms of the coefficients in the tableau (4).

Section 2 and the final section, 7, are technical. Section 7 contains the proofs of some lemmata. In section 2 we provide a brief description of NB-series [14]. These generalize to the decomposed case (1)–(2) the concept of B-series for undecomposed systems. B-series were introduced by Hairer and Wanner [13] and play a major role in studying the consistency properties of one-step integrators. In connection with Hamiltonian problems, B-series were first considered by Calvo and Sanz-Serna [6], who gave a necessary and sufficient condition for a B-series to be symplectic. These authors then showed how their general B-series result implies the known characterization of symplectic Runge–Kutta methods [15], [19], [23]. The B-series approach is particularly helpful when proving the necessity of symplecticness conditions; the alternative necessity proofs (see, e.g., [1]) are terribly messy. Also, [6] provided the basis for the proof of nonexistence of higher-derivative symplectic Runge–Kutta schemes [11]. The present paper provides an extension of the main result of [6] to the decomposed scenario; however, the technique of proof used here is different from those used in [6]. It should also be pointed out that a *partial* extension of [6] already exists: Murua [17], [18] and Hairer [10] have considered symplectic P-series; these are the particular case of NB-series corresponding to the situation where the decomposition (2) arises from partitioning the components into coordinates and momenta. As point out before, the P-series case is not just the particular case $N = 2$ of the NB-series theory.

2. Preliminaries.

2.1. *N*-trees.

We denote by D the dimension of (1) and use superscripts to refer to the components of y, f, $f^{[\nu]}$, e.g., $y = (y^1, y^2, \dots, y^D)^T$. Unless otherwise explicitly stated, f and the parts $f^{[\nu]}$ are supposed to be smooth and defined in the whole of $\mathcal{R}^D$.

N-trees provide a convenient tool to deal with the Taylor expansion of the solutions of (1) in terms of the $f^{[\nu]}$. From (1), for $i = 1, \dots, D$,

$$\begin{aligned}\frac{d^2 y^i}{dt^2} &= \sum_{\nu=1}^{N} f_j^{[\nu]i}(y)\frac{dy^j}{dt}\\ &= \sum_{\nu,\mu=1}^{N} f_j^{[\nu]i}(y) f^{[\mu]j}(y).\end{aligned} \tag{11}$$

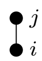
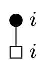
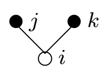
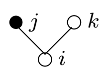
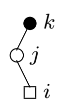
Here and later, subscripts denote partial differentiation, and we use Einstein's convention of summation on repeated indices. In turn, time differentiation in (11) leads to

$$\begin{aligned}\frac{d^3 y^i}{dt^3} &= \sum_{\nu,\mu=1}^{N} f_{jk}^{[\nu]i}(y)\frac{dy^k}{dt} f^{[\mu]j}(y)\\ &\quad+ \sum_{\nu,\mu=1}^{N} f_j^{[\nu]i}(y) f_k^{[\mu]j}(y)\frac{dy^k}{dt}\\ &= \sum_{\nu,\mu,\lambda=1}^{N} f_{jk}^{[\nu]i}(y) f^{[\lambda]k}(y) f^{[\mu]j}(y)\\ &\quad+ \sum_{\nu,\mu,\lambda=1}^{N} f_j^{[\nu]i}(y) f_k^{[\mu]j}(y) f^{[\lambda]k}(y).\end{aligned} \tag{12}$$

The terms being summed in expressions like (11) or (12) are easily described by means of N-trees. An N-tree is a tree where each vertex has been assigned, out of a

Table 1

Examples of 3-trees. The first, second, and third colors, respectively, correspond to black circles, white circles, and white squares.

N-tree	Elementary differential	ρ	α	σ	γ
$\emptyset$	y^i	0	1	1	1
	$f^{[1]i}$	1	1	1	1
	$f^{[2]i}$	1	1	1	1
	$f^{[3]i}$	1	1	1	1
	$f_j^{[1]i} f^{[1]j}$	2	1	1	2
	$f_j^{[1]i} f^{[2]j}$	2	1	1	2
	$f_j^{[3]i} f^{[1]j}$	2	1	1	2
	$f_{jk}^{[2]i} f^{[1]j} f^{[1]k}$	3	1	2	3
	$f_{jk}^{[2]i} f^{[1]j} f^{[2]k}$	3	2	1	3
	$f_j^{[3]i} f_k^{[2]j} f^{[1]k}$	3	1	1	6

choice of N, a color or type. For a full description of N-trees we refer to [9] or [17], where they are called P-trees and used in the particular case of decomposition by coordinate partitioning. When $N = 1$ all vertices are of the same color and we then identify 1-trees with the standard (uncolored) trees used in connection with Runge–Kutta methods [4], [12]. Note that throughout the paper, the terms tree and N-tree are always assumed to refer to *rooted* graphs; we use the terms free tree and free N-tree to refer to the cases without a root, i.e.; to the cases where no vertex has been highlighted. Table 1 contains, for the case $N = 3$, some examples of N-trees and the terms in (2), (11)–(12) that correspond to them.

We respectively denote by NT, $\overline{NT}$, $\overline{NT}^{[\nu]}$ the sets of N-trees, nonempty N-trees, and nonempty N-trees with root of color ν. The order $\rho(u)$ of the N-tree u is the number of vertices in u. The N-tree with a single vertex of type ν is denoted by $\tau^{[\nu]}$. Each N-tree with $\rho(u) > 1$ may be expressed in terms of nonempty N-trees of order $< \rho(u)$ as follows: we write

$$u = [u_1, \dots, u_m]^{[\nu]} \tag{13}$$

if the root of u is of color ν and $\{u_1, \ldots, u_m\}$ is the collection of N-trees arising from chopping off the root of u.

If $u \in \overline{NT}$ and $v \in NT$, we denote their Butcher product by $u \cdot v$. This is defined by (i) $u \cdot \emptyset = u$, (ii) $\tau^{[\nu]} \cdot v = [v]^{[\nu]}$ if $v \neq \emptyset$, and (iii) $u \cdot v = [u_1, \ldots, u_m, v]^{[\nu]}$ if u is as in (13) and $v \neq \emptyset$.

If u is as in (13) and $v \in \overline{NT}$, we denote by $k(u, v)$ the number of times that v appears amongst the u_i. Furthermore, we set $k(\tau^{[\nu]}, v) = 0$ for $\nu = 1, \ldots, N$ and $v \in \overline{NT}$. We also introduce the convention $k(u, \emptyset) = 1$ for each $u \in \overline{NT}$.

For $u \in NT$ we respectively denote by $\alpha(u)$, $\sigma(u)$ the number of monotonic labelings and symmetries of u. The definitions of these quantitites are straightforward extensions of those used for standard trees [4], [12]. Table 1 contains some values of α, σ; note, in particular in the last rows, that α and σ take into account the colors of the vertices. These functions may be recursively computed through the easily derived formulae [17]

$$\alpha(u \cdot v) = \frac{1}{k(u \cdot v, v)} \begin{pmatrix} \rho(u \cdot v) - 1 \\ \rho(v) \end{pmatrix} \alpha(u)\alpha(v) \tag{14}$$

and

$$\sigma(u \cdot v) = k(u \cdot v, v)\sigma(u)\sigma(v), \tag{15}$$

which relate the values at $u \cdot v$ to the values at the smaller N-trees u, v.

The density γ is defined by $\gamma(\emptyset) = \gamma(\tau^{[\nu]}) = 1$ and

$$\gamma(u) = \rho(u)\gamma(u_1) \cdots \gamma(u_m) \tag{16}$$

for u in (13). From (16) it follows that

$$\gamma(u \cdot v) = \frac{\rho(u) + \rho(v)}{\rho(u)} \gamma(u)\gamma(v), \tag{17}$$

and from (14)–(15) and (17) it is easily concluded by induction on the order $\rho(u)$ that

$$\rho(u)! = \alpha(u)\gamma(u)\sigma(u). \tag{18}$$

2.2. Elementary differentials. Given the system (1) *with the decomposition* (2), to each N-tree $u \in NT$, there corresponds an elementary differential $F(u)$. This is a mapping $\mathcal{R}^D \to \mathcal{R}^D$ recursively defined as follows:

$$F^i(\emptyset)(y) = y^i,$$
$$F^i(\tau^{[\nu]})(y) = f^{[\nu]i}(y)$$

and, for u in (13),

$$F^i(u)(y) = f^{[\nu]i}_{i_1, \ldots, i_m}(y) F^{i_1}(u_1)(y) \cdots F^{i_m}(u_m)(y). \tag{19}$$

In terms of elementary differentials, the derivatives of a solution $y(t)$ of (1) are given by

$$\frac{d^n y(t)}{dt^n} = \sum_{\substack{u \in NT \\ \rho(u) = n}} \alpha(u) F(u)(y(t))$$

(cf. (11)–(12)). Hence the Taylor expansion of $y(t+h)$ is

$$\sum_{u\in NT} \frac{h^{\rho(u)}}{\rho(u)!}\alpha(u)F(u)(y(t)),$$

or, using (18),

$$\sum_{u\in NT} \frac{h^{\rho(u)}}{\sigma(u)}\frac{1}{\gamma(u)}F(u)(y(t)). \tag{20}$$

2.3. NB-series. If $\mathbf{c}$ is a mapping that assigns to each $u \in NT$ a real number $\mathbf{c}(u)$, then an NB-series *relative to the decomposition* (2) is a formal power series

$$NB(\mathbf{c}, y) = \sum_{u\in NT} \frac{h^{\rho(u)}}{\sigma(u)}\mathbf{c}(u)F(u)(y). \tag{21}$$

For instance, the Taylor expansion (20) is $NB(\mathbf{c}, y(t))$ with $\mathbf{c}(u) = 1/\gamma(u)$ for each u.

In the particular case where the number N of parts in (2) is 1 (so that f is not really decomposed), an NB-series is a B-series:

$$B(\mathbf{c}, y) = \sum_{u\in T} \frac{h^{\rho(u)}}{\sigma(u)}\mathbf{c}(u)F(u)(y), \tag{22}$$

where $T = 1T$ is the set of trees with just one type of vertex. Note that (22) differs in the normalization of the coefficients from the standard definition of B-series [12]:

$$B^*(\mathbf{c}, y) = \sum_{u\in T} \frac{h^{\rho(u)}}{\rho(u)!}\alpha(u)\mathbf{c}(u)F(u)(y).$$

We have found that the normalization in this paper leads to simpler formulae than the standard normalization.

Each B-series (22) for the undecomposed system (1) induces an NB-series relative to the decomposition (2). For instance, the term

$$h\mathbf{c}(\cdot)F^i(\cdot)(y) = h\mathbf{c}(\cdot)f^i(y) = h\mathbf{c}(\cdot)\sum_{\nu=1}^{N} f^{[\nu]i}(y)$$

in the B-series gives rise in the induced NB-series to N terms

$$h\mathbf{c}(\bullet)f^{[\nu]i}(y), \qquad h\mathbf{c}(\circ)f^{[\nu]i}(y), \qquad \dots,$$

with $\mathbf{c}(\bullet) = \mathbf{c}(\circ) = \cdots = \mathbf{c}(\cdot)$. In a similar manner, the term

$$h^2\mathbf{c}(\overset{\cdot}{\underset{\cdot}{|}})F^i(\overset{\cdot}{\underset{\cdot}{|}})(y) = h^2\mathbf{c}(\overset{\cdot}{\underset{\cdot}{|}})f^i_j(y)f^j(y) = h^2\mathbf{c}(\overset{\cdot}{\underset{\cdot}{|}})\sum_{\nu,\mu=1}^{N} f_j^{[\nu]i}(y)f^{[\mu]j}(y)$$

gives rise to N^2 terms

$$h^2\mathbf{c}(\overset{\bullet}{\underset{\bullet}{|}})f_j^{[1]i}(y)f^{[1]j}(y), \qquad h^2\mathbf{c}(\overset{\circ}{\underset{\bullet}{|}})f_j^{[1]i}(y)f^{[2]j}(y), \qquad \dots,$$

with $\mathbf{c}\big(\substack{\bullet\\|\\\bullet}\big) = \mathbf{c}\big(\substack{\circ\\|\\\bullet}\big) = \cdots = \mathbf{c}\big(\substack{\bullet\\|\\\bullet}\big)$. The following result is not difficult to prove. It identifies the set of B-series for the (undecomposed) system (1) with a subset of the set of NB-series relative to a given decomposition (2).

THEOREM 1. *Given the system* (1)*, each* B*-series* $B(\mathbf{c}, y)$ *induces an* NB*-series* $NB(\mathbf{c}^*, y)$ *relative to the decomposition* (2) *in such a way that* $NB(\mathbf{c}^*, y) = B(\mathbf{c}, y)$ *for all* y*. The coefficients* $\mathbf{c}^*(u)$ *are given by* $\mathbf{c}^*(u) = \mathbf{c}(\overline{u})$*, where* $\overline{u} \in T$ *is the tree that one obtains from* $u \in NT$ *by ignoring the colors of the vertices.*

Conversely, if an NB*-series* $NB(\mathbf{c}^*, y)$ *relative to the decomposition* (2) *is such that* $\mathbf{c}^*(u) = \mathbf{c}^*(v)$ *whenever* u *and* v *only differ in the color of the vertices* ($\overline{u} = \overline{v}$)*, then* $NB(\mathbf{c}^*, y)$ *coincides with a* B*-series for the undecomposed system* (1)*.*

It turns out that, for virtually all one-step numerical methods for (1)–(2), the Taylor expansion in powers of h of the approximation y_{n+1} at time $t_{n+1} = t_n + h$ is given by an NB-series $NB(\mathbf{c}, y_n)$, where the coefficients $\mathbf{c}$ only depend on the numerical method. We illustrate how to obtain these coefficients in the case of ARK_N methods. Assume that the stage vectors $Y_{n,i}$ and the vectors $hf^{[\nu]}(Y_{n,i})$ have expansions respectively given by the NB-series $NB(\mathbf{d}_i, y_n)$ and $NB(\mathbf{g}_i^{[\nu]}, y_n)$. From (5) and (6) we respectively obtain, for $u \in \overline{NT}$,

$$\mathbf{d}_i(u) = \sum_{\nu=1}^{N} \sum_{j=1}^{s} a_{ij}^{[\nu]} \mathbf{g}_j^{[\nu]}(u), \qquad i = 1, \ldots, s, \tag{23}$$

$$\mathbf{c}(u) = \sum_{\nu=1}^{N} \sum_{i=1}^{s} b_i^{[\nu]} \mathbf{g}_i^{[\nu]}(u). \tag{24}$$

In turn, the $\mathbf{g}_i^{[\nu]}(u)$ may be expressed in terms of the $\mathbf{d}_i(v)$, with $\rho(v) < \rho(u)$ as follows (δ is the Kronecker symbol):

$$\mathbf{g}_i^{[\mu]}(\tau^{[\nu]}) = \delta_{\nu,\mu} \tag{25}$$

and, for u in (13),

$$\mathbf{g}_i^{[\mu]}(u) = \delta_{\nu,\mu} \prod_{k=1}^{m} \mathbf{d}_i(u_k). \tag{26}$$

These formulae can be used recursively to find the $\mathbf{c}(u)$ in terms of the coefficients $a_{ij}^{[\nu]}$, $b_i^{[\nu]}$ in the tableau (4). The same recursion may be applied to prove the fact that the Taylor expansions of $Y_{n,i}$ and $hf^{[\nu]}(Y_{n,i})$ are, in fact, B-series, something that was assumed in the derivation of the formulae above.

3. Symplectic NB-series.

3.1. The case of Hamiltonian parts.

Assume that (1) is a Hamiltonian system, i.e., that D is even $D = 2d$ and that there exists a real-valued function $H(y)$ such that

$$f(y) = J^{-1} \frac{\partial H}{\partial y}(y), \tag{27}$$

where $\partial H/\partial y = (\partial H/\partial y^1, \ldots, \partial H/\partial y^{2d})^T$ and J is the $2d \times 2d$ matrix

$$J = \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix}.$$

A transformation $\psi : \mathcal{R}^{2d} \to \mathcal{R}^{2d}$ is symplectic if its Jacobian ψ' satisfies

$$\psi'(y)^T J \psi'(y) = J. \tag{28}$$

We shall find conditions on the coefficients $\mathbf{c}(u)$ of the NB-series $NB(\mathbf{c}, y)$ for it to be symplectic, i.e., for (28) to hold for all y (in the sense of formal power series) for each decomposition (2) and each Hamiltonian system (1), (27).

We first look at the situation where the individual parts are themselves Hamiltonian:

$$f^{[\nu]}(y) = J^{-1} \frac{\partial H^{[\nu]}}{\partial y}(y), \tag{29}$$

with

$$H(y) = \sum_{\nu=1}^{N} H^{[\nu]}(y). \tag{30}$$

THEOREM 2. *Consider a sequence of coefficients* $\mathbf{c}$ *with* $\mathbf{c}(\emptyset) = 1$. *Then, the corresponding* NB*-series is symplectic for arbitrary Hamiltonian problems* (1), (27) *arbitrarily decomposed in Hamiltonian parts* (2), (29)–(30) *if and only if for each pair of nonempty* N*-trees*

$$\mathbf{c}(u \cdot v) + \mathbf{c}(v \cdot u) = \mathbf{c}(u)\mathbf{c}(v). \tag{31}$$

The proof uses a series of lemmata. We begin by associating with each $u \in \overline{NT}$ a matrix-valued function $F^*(u)(y)$ of the variable y. The (i, j) entry $F_j^{*i}(u)(y)$ of $F^*(u)(y)$ is recursively defined as follows (cf. the definition of the vector-valued elementary differentials in (19)). For $\nu = 1, \dots, N$,

$$F_j^{*i}(\tau^{[\nu]})(y) = f_j^{[\nu]i}(y)$$

and, if u is the N-tree in (13),

$$F_j^{*i}(u)(y) = f_{j,i_1,\dots,i_m}^{[\nu]i} F^{i_1}(u_1)(y) \cdots F^{i_m}(u_m)(y).$$

The matrices $F^*(u)(y)$ allow the recursive computation of the Jacobian matrices $F'(u)(y)$.

LEMMA 1. *Given a (not necessarily Hamiltonian) system* (1), *a decomposition* (2), *and a nonempty* N*-tree* u, *the following equalities between matrix-valued functions of* y *hold:*

$$\begin{aligned} F'(u) &= F^*(u) + \sum_{\substack{w_1, w_2 \in \overline{NT} \\ w_1 \cdot w_2 = u}} k(u, w_2) F^*(w_1) F'(w_2) \\ &= \sum_{\substack{w_1 \in \overline{NT}, w_2 \in NT \\ w_1 \cdot w_2 = u}} k(u, w_2) F^*(w_1) F'(w_2). \end{aligned} \tag{32}$$

Proof. Differentiate (19) with respect to y^j. Differentiation in the first factor $f_{i_1,\dots,i_m}^{[\nu]}(y)$ gives rise to the (i, j) entry of $F^*(u)(y)$. Differentiation in the second factor $F^{i_1}(u_1)(y)$ gives rise to the (i, j) entry of $F^*(w_1)(y)F'(w_2)(y)$ with $w_2 = u_1$, $w_1 = [u_2, \dots, u_m]^{[\nu]}$, etc. $\square$

LEMMA 2. *Assume that the right-hand side f of the Hamiltonian system* (1), (27) *has been decomposed in Hamiltonian parts as in* (2), (29)–(30). *Then, for each nonempty N-tree u, the following equality between matrix-valued functions of y holds:*

$$F^*(u)^T J + JF^*(u) = 0. \tag{33}$$

Proof. Since J is skew symmetric, $(JF^*(u))^T \equiv -F^*(u)^T J$, and we have to prove that $JF^*(u)(y)$ is symmetric. The (α, ω) entry of $JF^*(u)(y)$ is

$$\left[J_{\alpha i} f^{[\nu] i}_{\omega, i_1, \ldots, i_m}(y)\right] F^{i_1}(u_1)(y) \cdots F^{i_m}(u_m)(y),$$

and it is sufficient to prove that the expression in square brackets is symmetric in α, ω. This symmetry is established by noting that from (29),

$$J_{\alpha i} f^{[\nu] i}_{\omega}(y) = \frac{\partial}{\partial y^\omega}(Jf^{[\nu]}(y))^\alpha = H^{[\nu]}_{\alpha\omega}(y). \qquad \square$$

LEMMA 3. *In the situation of Lemma* 2, *for each nonempty N-tree z, the following equalities between matrix-valued functions of y hold:*

$$\sum_{\substack{u \in \overline{NT}, v \in NT \\ u \cdot v = z}} k(u \cdot v, v)[F'(u)^T JF'(v) + F'(v)^T JF'(u)] = 0, \tag{34}$$

$$F'(z)^T J + JF'(z) = -\sum_{\substack{u, v \in \overline{NT} \\ u \cdot v = z}} k(u \cdot v, v)[F'(u)^T JF'(v) + F'(v)^T JF'(u)]. \tag{35}$$

Proof. Clearly, (35) is a rewriting of (34). Let us use (32) in the left-hand side of (34) to get

$$\begin{aligned} &\sum_{\substack{w_1 \in \overline{NT}, w_2, v \in NT \\ (w_1 \cdot w_2) \cdot v = z}} k(z, v) k(w_1 \cdot w_2, w_2) \\ &\quad \times \left[F'(w_2)^T F^*(w_1)^T JF'(v) + F'(v)^T JF^*(w_1) F'(w_2)\right]. \end{aligned} \tag{36}$$

Note that $k(z, v)k(w_1 \cdot w_2, w_2)$ is not altered by swapping v and w_2: this is obvious if $v = w_2$, while for $v \neq w_2$

$$k(z, v) = k((w_1 \cdot w_2) \cdot v, v) = k(w_1 \cdot v, v)$$

and

$$k(w_1 \cdot w_2, w_2) = k((w_1 \cdot w_2) \cdot v, w_2) = k(z, w_2).$$

Therefore, (36) may be rewritten as

$$\sum_{\substack{w_1 \in \overline{NT}, w_2, v \in NT \\ (w_1 \cdot w_2) \cdot v = z}} k(z, v) k(w_1 \cdot w_2, w_2) F'(w_2)^T \left[F^*(w_1)^T J + JF^*(w_1)\right] F'(v),$$

an expression that vanishes in view of (33). $\square$

LEMMA 4. *Consider an* NB*-series* $NB(\mathbf{c}, y)$ *with* $\mathbf{c}(\emptyset) = 1$ *relative to a decomposition* (2) *of the (not necessarily Hamiltonian) two-dimensional problem* (1). *If we set* $\psi(y) = NB(\mathbf{c}, y)$, *then the following equality of functions of* y *holds:*

$$\psi'^T J\psi' - J = \sum_{\substack{u,v\in NT\\(u,v)\neq(\emptyset,\emptyset)}} \frac{h^{\rho(u)}}{\sigma(u)}\frac{h^{\rho(v)}}{\sigma(v)}\mathbf{c}(u)\mathbf{c}(v)F'(u)^T JF'(v). \tag{37}$$

If, furthermore, the system (1) *is Hamiltonian* (27) *and has been decomposed in Hamiltonian parts as in* (2), (29)–(30), *then*

$$\psi'^T J\psi' = \sum_{u,v\in\overline{NT}} \frac{h^{\rho(u)}}{\sigma(u)}\frac{h^{\rho(v)}}{\sigma(v)}[\mathbf{c}(u)\mathbf{c}(v) - \mathbf{c}(u\cdot v) - \mathbf{c}(v\cdot u)]F'(u)^T JF'(v). \tag{38}$$

Proof. The formula (37) is an obvious consequence of (21).

On separating the case where one of u, v is empty, we obtain from (37)

$$\begin{aligned}\psi'^T J\psi' = &\sum_{z\in\overline{NT}} \frac{h^{\rho(z)}}{\sigma(z)}\mathbf{c}(z)[F'(z)^T J + JF'(z)]\\ &+ \sum_{u,v\in\overline{NT}} \frac{h^{\rho(u)}}{\sigma(u)}\frac{h^{\rho(v)}}{\sigma(v)}\mathbf{c}(u)\mathbf{c}(v)F'(u)^T JF'(v).\end{aligned} \tag{39}$$

We now use (35) to rewrite the first sum in (39) in the form

$$-\sum_{u,v\in\overline{NT}} \frac{h^{\rho(u\cdot v)}}{\sigma(u\cdot v)}k(u\cdot v, v)\mathbf{c}(u\cdot v)[F'(u)^T JF'(v) + F(v)^T JF'(u)]. \tag{40}$$

Then (38) is a consequence of (15). ◻

It is obvious that the theorem is a consequence of formula (38), in view of the following result whose proof is given in the final section.

LEMMA 5. *Given* $u, v \in \overline{NT}$ *there exists a polynomial Hamiltonian function* H *with* $d = \rho(u) + \rho(v) + 1$ *degrees of freedom and a Hamiltonian decomposition* (30) *such that, if* $w, z \in \overline{NT}$, *the entry* $(1, d + 2)$ *of* $F'(w)^T(0)JF'(z)(0)$ *is nonzero if and only if* $z = u$ *and* $w = v$.

3.2. The case of general parts. In this subsection f is Hamiltonian, so that (27) holds, but the parts $f^{[\nu]}$ themselves are not assumed to be Hamiltonian (i.e., (29) does not necessarily hold). Since we now demand symplecticness for more general decompositions, it is expected that (31), while still being necessary, is no longer sufficient. In fact, we have the following result.

THEOREM 3. *Consider a sequence of coefficients* $\mathbf{c}$ *with* $\mathbf{c}(\emptyset) = 1$. *Then the following statements are equivalent.*

(i) *The* NB*-series* $NB(\mathbf{c}, \cdot)$ *is symplectic for all Hamiltonian systems* (1), (27) *and all decompositions* (2) *(with not necessarily Hamiltonian parts).*

(ii) *For each pair of nonempty* N*-trees* w, z,

$$\mathbf{c}(w\cdot z) + \mathbf{c}(z\cdot w) = \mathbf{c}(w)\mathbf{c}(z), \tag{41}$$

and for each pair of nonempty N*-trees* u, v *that only differ in the color of their roots*

$$\mathbf{c}(u) = \mathbf{c}(v). \tag{42}$$

(iii) *The* NB-*series* $NB(\mathbf{c}, y)$ *is equivalent in the sense in Theorem* 1 *to a symplectic* B-*series.*

Note that by (iii) it is impossible to have genuinely symplectic methods for decomposed systems if the parts $f^{[\nu]}$ are arbitrary: a symplectic method for the decomposed system can always be rewritten as a symplectic method for the undecomposed system.

Proof. We succesively show that (i) $\Rightarrow$ (ii), (ii) $\Rightarrow$ (iii), (iii) $\Rightarrow$ (i).

Assume that $NB(\mathbf{c}, y)$ is symplectic as in (i). Then, by Theorem 2, (41) holds. That (42) also holds follows, in view of (37), from Lemma 6 below.

Now assume that (ii) holds. We show that $NB(\mathbf{c}, y)$ is induced by a B-series, i.e., that $\mathbf{c}(u_1) = \mathbf{c}(u_2)$ if u_1 and u_2 only differ in the coloring of the vertices. It is clearly sufficient to consider the case where u_1, u_2 only differ in the color of *one* vertex. If this vertex is the root, then $\mathbf{c}(u_1) = \mathbf{c}(u_2)$ by (42). If the vertex that is colored differently in u_1, u_2 is a son of the root, then $u_1 = v \cdot w_1$, $u_2 = v \cdot w_2$, with w_1 and w_2 differing only in the color of their roots. Then by (41), for $i = 1, 2$,

$$\mathbf{c}(u_i) = -\mathbf{c}(w_i \cdot v) + \mathbf{c}(v) + \mathbf{c}(w_i),$$

and the right-hand side of this expression does not depend on i because the pairs $w_1 \cdot v$, $w_2 \cdot v$ and w_1, w_2 only differ in the color of their roots. Hence $\mathbf{c}(u_1) = \mathbf{c}(u_2)$. If the vertex that is colored differently in u_1, u_2 is a son of a son of the root, then $u_1 = v \cdot (w \cdot z_1)$, $u_2 = v \cdot (w \cdot z_2)$, with z_1 and z_2 differing only in the color of their roots. From

$$\mathbf{c}(u_i) = -\mathbf{c}((w \cdot z_i) \cdot v) + \mathbf{c}(v) + \mathbf{c}(w \cdot z_i),$$

we conclude that $c(u_1) = c(u_2)$ because the pairs $(w \cdot z_1) \cdot v$, $(w \cdot z_2) \cdot v$ and $w \cdot z_1$, $w \cdot z_2$ only differ in the color of a son of their roots. By carrying on with this procedure we show that $NB(\mathbf{c}, y)$ is in fact a B-series $B(\mathbf{d}, y)$. By (41) the coefficients of this B-series satisfy the sufficient symplecticness condition in Theorem 2.

The implication (iii) $\Rightarrow$ (i) is trivial. ∎

The next lemma, whose proof is given in the final section, was required in the proof of the theorem when showing that (42) follows from the symplecticness of $NB(\mathbf{c}, y)$.

LEMMA 6. *Given two nonempty N-trees u, v differing only in the color of their roots, there exists a polynomial Hamiltonian function H with $d = \rho(u) + 1$ degrees of freedom and a decomposition* (2) *in non-Hamiltonian parts such that, if $w, z \in NT$, then the $(1, d+2)$ entry of $F'(w)^T(0)JF'(z)(0)$ is zero if and only if either $w = \emptyset$, $z = v$ or $w = u$, $z = \emptyset$. Furthermore,*

$$[JF'(v)(0)]_{1,d+2} = -\left[F'(u)^T(0)J\right]_{1,d+2}.$$

In the proof of the theorem we have showed *indirectly* that (41) and (42) are necessary and sufficient for $NB(\mathbf{c}, y)$ to be symplectic. A direct argument, along the lines of the proof of Theorem 2, will now be presented in view of the insight it provides.

Lemma 1 still applies to the present situation where the parts are not assumed to be Hamiltonian. Lemma 2 does not. However, f is Hamiltonian and the proof of Lemma 2 is valid with f replacing $f^{[\nu]}$. This shows that the conclusion of Lemma 2 holds provided that we sum in ν. More precisely, we have the following lemma.

LEMMA 7. *Assume that the right-hand side f of the Hamiltonian system* (1), (27) *has been decomposed in not necessarly Hamiltonian parts as in* (2). *Then, for each* *nonempty N-tree u,*

$$\sum_{\nu=1}^{N}[F^*(u^{[\nu]})^T J + JF^*(u^{[\nu]})] = 0,$$

where $u^{[\nu]}$ denotes the N-tree obtained from u by painting the root of u with the νth color.

In turn, the following lemma, which again includes a summation in ν, replaces Lemma 3.

LEMMA 8. *In the situation of Lemma* 7, *for each nonempty N-tree z,*

$$\begin{aligned}&\sum_{\nu=1}^{N}[F'(u^{[\nu]})^T J + JF'(u^{[\nu]})]\\ &\quad = -\sum_{\nu=1}^{N}\sum_{\substack{u,v\in\overline{NT}\\ u\cdot v=z^{[\nu]}}} k(u\cdot v, v)\left[F'(u)^T JF'(v) + F'(v)^T JF'(u)\right].\end{aligned}$$

Finally, we show that (38), leading to the equivalence of (i) in the theorem and (41), still holds. However, to carry our argument through, we need (42) in order to be able to take $\mathbf{c}(z^{[\nu]})$ as a common factor in the summation over colors.

LEMMA 9. *In the situation of Lemma* 7 *assume that $\mathbf{c}(u) = \mathbf{c}(v)$ whenever u and v differ only in the color of their roots. Then* (38) *holds.*

Proof. Since $\rho(z)$, $\sigma(z)$, and $\mathbf{c}(z)$ do not change their values when the color of the root of z is changed, we may rewrite the right-hand side of (39) in the form

$$\begin{aligned}&\sum_{z\in\overline{NT}^{[1]}} \frac{h^{\rho(z)}}{\sigma(z)}\mathbf{c}(z)\sum_{\nu=1}^{N}[F'(z^{[\nu]})^T J + JF'(z^{[\nu]})]\\ &\quad + \sum_{u,v\in\overline{NT}} \frac{h^{\rho(u)}}{\sigma(u)}\frac{h^{\rho(v)}}{\sigma(v)}\mathbf{c}(u)\mathbf{c}(v)F'(u)^T JF'(v).\end{aligned}$$

By Lemma 8, the first summation equals (40). After this, the proof is identical to that of Lemma 4. $\square$

4. Order conditions for symplectic NB-series. Assume that a numerical method for the, not necessarily Hamiltonian, problem (1)–(2) is such that the expansion of y_{n+1} is an NB-series $NB(\mathbf{c}, y_n)$ for a method-dependent sequence of coefficients $\mathbf{c}(u)$ with $\mathbf{c}(\emptyset) = 1$. Then, by comparing the NB-series for the true and numerical solutions, we conclude that the conditions

$$\mathbf{c}(u) = \frac{1}{\gamma(u)}, \qquad 1 \le \rho(u) \le r, \tag{43}$$

are *sufficient* for the method to be consistent of order r. The conditions (43) are also necessary to have order r for arbitrary (1)–(2), because the elementary differentials are independent, as shown by the following result to be proved in the final section.

LEMMA 10. *Given a nonempty N-tree u, there exists a polynomial Hamiltonian H with $d = \rho(u)$ degrees of freedom and a decomposition* (2) *in Hamiltonian parts* (29)–(30) *such that if $v \in \overline{NT}$, then $F^1(v)(0) \neq 0$ if and only if $v = u$.*

The fact that in this lemma the problem being integrated can be chosen to be Hamiltonian with a Hamiltonian decomposition implies that the order of an NB-series method when applied to arbitrary Hamiltonian decompositions of arbitrary Hamiltonian right-hand sides is not higher than when applied to arbitrary non-Hamiltonian right-hand sides. In other words, the order of consistency of a method is not increased by restricting the attention to Hamiltonian problems with Hamiltonian decomposition. (It is, on the other hand, well known that the order of a method is in general higher for scalar problems, than for general problems, because for scalar problems, not all elementary differentials are independent; see, e.g., [5].)

Now assume that the symplecticness condition (31) is satisfied. Then, it is expected that the order conditions in (43) are not all independent. This was first noticed for Runge–Kutta methods in [21] and is a consequence of the fact that symplectic transformations possess a scalar generating function [22] or may be expressed in terms of a modified Hamiltonian function [22], [10]. From (17), if $u, v \in \overline{NT}$, then

$$\frac{1}{\gamma(u\cdot v)} + \frac{1}{\gamma(v\cdot u)} = \frac{1}{\gamma(u)}\frac{1}{\gamma(v)}. \tag{44}$$

Therefore, if the symplecticness condition (31) holds and the order conditions for the N-trees u and v are satisfied, then the order conditions for $u\cdot v$ and $v\cdot u$ are equivalent.

It is convenient to introduce in $\overline{NT}$ an equivalence relation $\sim$ defined as the finest equivalence relation such that $u\cdot v$ and $v\cdot u$ are in the same equivalence class for $u, v \in \overline{NT}$ (finest equivalence relation means the equivalence relation with smallest equivalence classes). Since, in the pictorial representation of N-trees, going from $u\cdot v$ to $v \cdot u$ corresponds to "moving the root one vertex away," it turns out that $u \sim v$ if and only if u and v only differ in the location of their roots, i.e., they are identical as free (unrooted) graphs. In other words, there is an equivalence class per nonempty free N-tree.

Following [21], we say that a free N-tree is *superfluous* if, when seen as an equivalence class of (rooted) N-trees, it contains an N-tree of the form $u \cdot u$. By taking $u = v$ in (44) and (31), we see that the order condition for $u\cdot u$ is implied by the order condition for u. Summing up, we have arrived at the following extension of Theorem 2.2 in [6].

THEOREM 4. *Suppose that an* NB*-series method possesses order of consistency* $\geq r-1$, $r \geq 2$ *and satisfies the symplecticness condition* (31). *Then the method has order* $\geq r$ *if (and only if) each nonsuperfluous free N-tree of order r contains an N-tree z for which the order condition* $\mathbf{c}(z) = 1/\gamma(z)$ *holds.*

A detailed counting of the number of order conditions for symplectic and general methods cannot be included here for reasons of brevity. The interested reader is referred to Araújo's forthcoming thesis.

5. Decompositions based on partitioning the components.

5.1. General Hamiltonians. For Hamiltonian system (1), (27) the components of y are naturally partitioned into two parts $y = (p^T, q^T)^T$, $p = (y^1, \ldots, y^d)^T$, $q = (y^{d+1}, \ldots, y^{2d})^T$. In applications to mechanics, the components p^i of p are momenta and the components q^i of q are coordinates. In view of this partition of y, we may partition f into two parts (cf. (7)):

$$f^{[1]i}(y) = f^i(y) = -\frac{\partial H(p,q)}{\partial q^i}, \quad i = 1, \ldots, d,$$

$$f^{[1]i}(y) = 0, \quad i = d+1, \ldots, 2d,$$

$$f^{[2]i}(y) = 0, \quad i = 1, \ldots, d,$$
$$f^{[2]i}(y) = f^i(y) = \frac{\partial H(p,q)}{\partial p^{i-d}}, \quad i = d+1, \ldots, 2d.$$

Note that the parts $f^{[1]}$, $f^{[2]}$ are *not Hamiltonian.* However, nontrivial symplectic integrators may exist (cf. Theorem 3). This is possible because, due to the block structure of $f^{[1]}$, $f^{[2]}$ and the matrix J,

$$F'(u)^T J F'(v) = 0, \quad u, v \in \overline{NT}^{[i]}, \quad i = 1, 2, \tag{45}$$

so that in (37) the terms where u and v have roots of the same color vanish. The second part of Lemma 4 is not applicable to investigating symplecticness, and we have to resort to the alternative Lemma 9, whose application requires that $\mathbf{c}(u) = \mathbf{c}(v)$ whenever u and v only differ in the color of their roots. We then obtain the "if" part of the following theorem.

THEOREM 5. *Let $N = 2$ and consider a sequence of coefficients $\mathbf{c}$ with $\mathbf{c}(\emptyset) = 1$. Then the corresponding* 2B*-series is symplectic for arbitrary Hamiltonian problems* (1), (27) *decomposed by (p,q)-partitioning if and only if the following conditions hold.*

(i) *If $u \in \overline{2T}^{[1]}$ and $v \in \overline{2T}^{[2]}$, then $\mathbf{c}(u \cdot v) + \mathbf{c}(v \cdot u) = \mathbf{c}(u)\mathbf{c}(v)$.*

(ii) *If $u \in \overline{2T}^{[1]}$ and $v \in \overline{2T}^{[2]}$ differ only in the color of their roots, then $\mathbf{c}(u) = \mathbf{c}(v)$.*

The "only if" part is shown by constructions similar to those used in the proofs of Lemmata 5 and 6; see [17] or [10].

To discuss the order conditions, Hairer [10] introduced an equivalence relation $\sim^*$ in $\overline{NT}$ defined as the finest equivalence relation for which (i) $u \cdot v \sim^* v \cdot u$ if $u \in \overline{2T}^{[1]}$ and $v \in \overline{2T}^{[2]}$, and (ii) $u \sim^* v$, if $u \in \overline{2T}^{[1]}$ and $v \in \overline{2T}^{[2]}$ differ only in the color of their roots. The equivalence relation $\sim$ in the preceding section is not finer (i.e., does not possess smaller equivalence classes) than $\sim^*$, because, when u and v have roots of the same color, $u \cdot v$ and $v \cdot u$ are $\sim$ related, but not necessarily $\sim^*$ related. But $\sim$ is not coarser than $\sim^*$ because if u and v differ only in the color of their roots, then they are $\sim^*$ related but not necessarily $\sim$ related. The identification of the $\sim^*$ equivalence classes with suitable graphs called H-trees is due to Murua [18]. A result similar to Theorem 4 holds with H-trees playing the role played there by nonsuperfluous N-trees.

5.2. Separable Hamiltonians. For the particular case of separable Hamiltonians,

$$H(p,q) = T(p) + V(q), \tag{46}$$

the (p,q)-partitioning leads to Hamiltonian parts $f^{[1]}$, $f^{[2]}$, and therefore this decomposition is covered by Theorem 2. The relation (45), of course, still applies, but furthermore, $f^{[1]}$ does not depend on p and $f^{[2]}$ does not depend on q, and this implies that $F(u) \equiv 0$ if $u \in \overline{2T}$ is such that two adjacent vertices possess the same color. It is then enough to consider the set $\overline{S2T}$ of special 2-trees comprising those 2-trees where the color of a son is the opposite of the color of its father. We then obtain the "if" part of the following theorem.

THEOREM 6. *Let $N = 2$ and consider a sequence of coefficients $\mathbf{c}$ with $\mathbf{c}(\emptyset) = 1$. Then the corresponding* 2B*-series is symplectic for arbitrary separable Hamiltonian problems* (1), (27), (46) *decomposed by (p,q)-partitioning if and only $\mathbf{c}(u \cdot v) + \mathbf{c}(v \cdot u) = \mathbf{c}(u)\mathbf{c}(v)$ for $u \in \overline{S2T}^{[1]}$ and $v \in \overline{S2T}^{[2]}$.*

The "only if" part requires a construction similar to that in Lemma 5 (see [17], [10]), this time involving a separable Hamiltonian.

To study the order conditions, an equivalence relation is introduced. This time, each equivalence class corresponds to a free special 2-tree, a tree without a root where the vertices have been painted with two colors in such a way that adjacent vertices receive different colors (these graphs are called bicolor (unrooted) trees in [22]). A result similar to Theorem 4 holds with free special 2-trees playing the role played there by nonsuperfluous N-trees.

6. Application to ARK Methods.

6.1. A sufficient condition for symplecticness.

We begin with sufficient conditions. Note the low smoothness required.

THEOREM 7. (i) *Assume that the system* (1) *is Hamiltonian with a general decomposition* (2)*, with* f*,* $f^{[\nu]}$ *of class* C^1 *in an open subset of* $\mathcal{R}^{2d}$*. Assume that, for a given* h*, the formulae* (5)–(6) *define a mapping* $\psi : y_n \mapsto y_{n+1}$ *in an open subset of* $\mathcal{R}^{2d}$*. Then the conditions*

$$b_i^{[\nu]} = b_i^{[\mu]}, \qquad i = 1, \ldots, s, \quad \mu, \nu = 1, \ldots, N, \tag{47}$$

and

$$b_i^{[\nu]} a_{ij}^{[\mu]} + b_j^{[\mu]} a_{ji}^{[\nu]} - b_i^{[\nu]} b_j^{[\mu]} = 0, \qquad i, j = 1, \ldots, s, \quad \mu, \nu = 1, \ldots, N, \tag{48}$$

are sufficient for ψ *to be a symplectic transformation.*

(ii) *If in* (i) *the parts* $f^{[\nu]}$ *are themselves Hamiltonian, then* (48)*, on its own, is sufficient for* ψ *to be symplectic.*

Proof. It is similar to the proof for Runge–Kutta and partitioned Runge–Kutta methods [22] and will not be given. ∎

We now describe the family of methods satisfying (48). It is possible to assume that if, for given i and ν, $b_i^{[\nu]} = 0$, then $a_{ji}^{[\nu]} = 0$ for each $j = 1, \ldots, s$. In fact, the conditions $b_i^{[\nu]} = 0$, $a_{ji}^{[\nu]} \neq 0$ substituted in (48) imply $b_j^{[\mu]} = 0$ for all μ, and then the stage $Y_{n,j}$ is not used by the method. Therefore, after suppressing redundant stages, we may parameterize the $a_{ij}^{[\nu]}$, $i, j = 1, \ldots, s$, $\nu = 1, \ldots, N$, in the form $a_{ij}^{[\nu]} = \lambda_{ij}^{[\nu]} b_j^{[\nu]}$; if $b_j^{[\nu]} \neq 0$, then $\lambda_{ij}^{[\nu]} = a_{ij}^{[\nu]} / b_j^{[\nu]}$, while for $b_j^{[\nu]} = 0$, the value of $\lambda_{ij}^{[\nu]}$ is of no consequence. With this parameterization (48) becomes

$$b_i^{[\nu]} b_j^{[\mu]} (\lambda_{ij}^{[\mu]} + \lambda_{ji}^{[\nu]} - 1) = 0, \qquad i, j = 1, \ldots, s, \quad \mu, \nu = 1, \ldots, N, \tag{49}$$

a system that possesses the family of solutions

$$\begin{aligned}
&b_i^{[\nu]} \quad \text{free}, \qquad i = 1, \ldots, s, \quad \nu = 1, \ldots, N, \\
&\lambda_{ii}^{[\nu]} = \frac{1}{2}, \qquad i = 1, \ldots, s, \quad \nu = 1, \ldots, N, \\
&\lambda_{ij}^{[\nu]} = \mu_{ij},, \qquad i, j = 1, \ldots, s, \quad j > i, \quad \nu = 1, \ldots, N, \\
&\lambda_{ij}^{[\nu]} = 1 - \mu_{ji},, \qquad i, j = 1, \ldots, s, \quad j < i, \quad \nu = 1, \ldots, N,
\end{aligned} \tag{50}$$

where μ_{ij}, $j > i$ are free parameters. It is not difficult to show that, for methods without redundant stages, (50) provides all solutions of (49), in the sense that other possible solutions are obtained from (50) by changing the value of the $\lambda_{ij}^{[\nu]}$'s for which the corresponding $b_j^{[\nu]}$ vanishes. In conclusion, for methods without redundant stages, the solutions of (48) are given by the following family with $sN + s(s-1)/2$ free parameters:

$$
\begin{aligned}
&b_i^{[\nu]} \quad \text{free}, \qquad i=1,\dots,s, \quad \nu=1,\dots,N,\\
&a_{ii}^{[\nu]} = \frac{b_i^{[\nu]}}{2}, \qquad i=1,\dots,s, \quad \nu=1,\dots,N,\\
&a_{ij}^{[\nu]} = b_j^{[\nu]}\mu_{ij},, \qquad i,j=1,\dots,s, \quad j>i, \quad \nu=1,\dots,N,\\
&a_{ij}^{[\nu]} = b_j^{[\nu]}(1-\mu_{ji}),, \qquad i,j=1,\dots,s, \quad j<i, \quad \nu=1,\dots,N.
\end{aligned}
\tag{51}
$$

All these methods are implicit. To obtain diagonally implicit methods with $a_{ij}^{[\nu]}=0$ for $j>i$, we have to set all the $\mu_{ij}=0$, and this leaves a family with sN free parameters. By choosing some of the $b_i^{[\nu]}$ to be zero, it is possible to gain favorable sparsity patterns, as examplified by method (10).

From (51), it is clear that a method that satisfies both (47) and (48) is equivalent to a symplectic standard Runge–Kutta method, as one may have conjectured from Theorem 3.

6.2. NB-series approach. After the sufficient condition in Theorem 7, we apply the results of section 2 to the investigation of *necessary* and sufficient conditions for the NB-series associated with an ARK_N method to be symplectic. The techniques are similar to those in [11]. We shall use the following lemma. An ARK_N is said to be S-reducible if it has two identical stages $Y_{n,i} \equiv Y_{n,j}$.

LEMMA 11. *For the ARK_N method* (4), *consider the $Ns \times \infty$ matrix G, whose columns are given by*

$$
\left(\mathbf{g}_1^{[1]}(u),\dots,\mathbf{g}_s^{[1]}(u);\dots;\mathbf{g}_1^{[N]}(u),\dots,\mathbf{g}_s^{[N]}(u)\right)^T, \tag{52}
$$

where u ranges over $\overline{NT}$. Then the method is S*-irreducible if and only if G has full rank Ns.*

Proof. If the method is not S-irreducible, then $s>1$ and there are indices i, j, $i \neq j$, such that $Y_{n,i} \equiv Y_{n,j}$ and hence $\mathbf{g}_i^{[\nu]}(u) = \mathbf{g}_j^{[\nu]}(u)$ for $u \in \overline{NT}$ and all ν. Then G has, at most, rank $N(s-1)$.

Assume now that the method is S-irreducible. We observe that (26) implies that if u has root of color ν, then the column vector (52) has 0 entries except for the block

$$
\left(\mathbf{g}_1^{[\nu]}(u),\dots,\mathbf{g}_s^{[\nu]}(u)\right)^T. \tag{53}
$$

Therefore, G has rank Ns if and only if each of the $s\times\infty$ matrices $G^{[\nu]}$ with columns (53) ($u \in \overline{NT}^{[\nu]}$) has full rank s. Fix $\nu = 1,\dots,N$. It is clear that it is sufficient to show that there exists an $\infty\times s$ matrix C with columns C_i, $i=0,\dots,s-1$, such that $G^{[\nu]}C$ is an invertible Vandermonde matrix.

Assume that the N-trees in $\overline{NT}^{[\nu]}$ have been ordered in such a way that the first column in $G^{[\nu]}$ corresponds to $\tau^{[\nu]}$. Then, by (25), the choice $C_0 = (1,0,0,\dots)^T$ ensures that the first column of $G^{[\nu]}C$ is the vector $(1,\dots,1)^T$. In point (i) below we show that C_1 can be chosen (with finitely many nonzero components) so that $G^{[\nu]}C_1 = (\eta_1,\dots,\eta_s)^T$ with $\eta_i \neq \eta_j$ for $i \neq j$. Finally, in point (ii) below, we show how to choose $C_2,\dots,C_{s-1}$ so that $G^{[\nu]}C_l = (\eta_1^\ell,\dots,\eta_s^\ell)^T$. This concludes the proof of the lemma.

(i) Since the method is S-irreducible, to each pair (i,j) with $i \neq j$, there corresponds $u \in \overline{NT}^{[\nu]}$ such that $\mathbf{d}_i(u) \neq \mathbf{d}_j(u)$. By (26),

$$\mathbf{g}_i^{[\nu]}([u]^{[\nu]}) = \mathbf{d}_i(u) \neq \mathbf{d}_j(u) = \mathbf{g}_j^{[\nu]}([u]^{[\nu]}).$$

It is clear that we may select finitely many constants α_k and N-trees $u_k \in \overline{NT}^{[\nu]}$ such that

$$\eta_i = \sum_k \alpha_k \mathbf{g}_i^{[\nu]}([u_k]^{[\nu]})$$

are such that $\eta_i \neq \eta_j$ for $i \neq j$.

(ii) Take the ℓth power of η_i:

$$\begin{aligned}\eta_i^\ell &= \Big(\sum_k \alpha_k \mathbf{g}_i^{[\nu]}([u_k]^{[\nu]})\Big)^\ell \\ &= \sum_{k_1,\dots,k_\ell=1} \alpha_{k_1}\cdots\alpha_{k_\ell}\mathbf{g}_i^{[\nu]}([u_{k_1}]^{[\nu]})\cdots\mathbf{g}_i^{[\nu]}([u_{k_\ell}]^{[\nu]}).\end{aligned}$$

According to (26),

$$\begin{aligned}\eta_i^\ell &= \sum_{k_1,\dots,k_\ell=1} \alpha_{k_1}\cdots\alpha_{k_\ell}\mathbf{d}_i(u_{k_1})\cdots\mathbf{d}_i(u_{k_\ell}) \\ &= \sum_{k_1,\dots,k_\ell=1} \alpha_{k_1}\cdots\alpha_{k_\ell}\mathbf{g}_i^{[\nu]}([u_{k_1},\cdots,u_{k_\ell}]^{[\nu]}). \qquad \square\end{aligned}$$

The next result shows that the condition (48), which has been proved to be sufficient for symplecticness in the case of Hamiltonian parts, is also necessary. Note that, in Theorem 2, (31) is necessary for symplecticness *in the sense of formal series* for *polynomial* Hamiltonians (see Lemma 5). For h small enough, the series actually converge, so that we shall in fact prove that (48) is necessary for the method to define a symplectic transformation when applied with small step-sizes to polynomial Hamiltonians decomposed in Hamiltonian parts. By implication, the family (51) comprises all irreducible symplectic ARK$_N$ methods.

THEOREM 8. *Assume that the ARK$_N$ method* (4) *is* S-*irreducible. Then the necessary and sufficient condition* (31) *for the symplecticness of the corresponding* NB-*series for arbitrary Hamiltonian systems* (1), (27) *decomposed in Hamiltonian parts* (2), (29)–(30) *is equivalent to* (48).

Proof. Denote by $m_{ij}^{[\nu,\mu]}$ the left-hand side of (48). If $u, v \in \overline{NT}$, then, by the definition of $m_{ij}^{[\nu,\mu]}$,

$$\begin{aligned}\sum_{i,j=1}^{s}\sum_{\nu,\mu=1}^{N} m_{ij}^{[\nu,\mu]}\mathbf{g}_i^{[\nu]}(u)\mathbf{g}_j^{[\mu]}(v) &= \sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(u)\mathbf{d}_i(v) \\ &\quad + \sum_{j=1}^{s}\sum_{\mu=1}^{N} b_j^{[\mu]}\mathbf{d}_j(u)\mathbf{g}_j^{[\mu]}(v) \\ &\quad - \Big(\sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(u)\Big)\Big(\sum_{j=1}^{s}\sum_{\mu=1}^{N} b_j^{[\mu]}\mathbf{g}_j^{[\mu]}(u)\Big).\end{aligned}$$

By (26), the right-hand side of this expression equals

$$\sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(u\cdot v) + \sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(v\cdot u)$$
$$-\left(\sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(u)\right)\left(\sum_{i=1}^{s}\sum_{\nu=1}^{N} b_i^{[\nu]}\mathbf{g}_i^{[\nu]}(u)\right),$$

which, by (24), coincides with

$$\mathbf{c}(u\cdot u) + \mathbf{c}(v\cdot u) - \mathbf{c}(u)\mathbf{c}(v).$$

Thus (31) is equivalent to $G^T MG = 0$, where M is the block matrix with blocks

$$M^{[\nu,\mu]} = \begin{bmatrix} m_{11}^{[\nu,\mu]} & \cdots & m_{1s}^{[\nu,\mu]} \\ \vdots & \ddots & \vdots \\ m_{s1}^{[\nu,\mu]} & \cdots & m_{ss}^{[\nu,\mu]} \end{bmatrix},$$

and G is as in the preceding lemma. If the method is S-irreducible, G has full rank and $G^T MG = 0$ if and only if $M = 0$. ◻

The last result in this section implies that if an ARK_N method defines a symplectic transformation when applied with small h to polynomial Hamiltonians decomposed in non-Hamiltonian parts, then (47) and (48) hold. As we discussed above, this in turn implies that the method is equivalent to a (symplectic) standard Runge–Kutta method.

THEOREM 9. *Assume that* (4) *is* S*-irreducible. Then the condition* (ii) *in Theorem* 3*, guaranteeing symplecticness for non-Hamiltonian parts, is equivalent to* (47)–(48).

Proof. After the preceding theorem we have to show that (47) and (42) are equivalent. We now introduce the quantities

$$p_j^{[\nu,\mu]} = b_j^{[\nu]} - b_j^{[\mu]}$$

and the matrix P with blocks

$$P^{[\nu,\mu]} = \begin{bmatrix} p_1^{[\nu,\mu]} & \cdots & p_s^{[\nu,\mu]} \end{bmatrix}.$$

By using techniques similar to those in the preceding proof it is possible to show that (42) is equivalent to $PG = 0$. Since G has full rank, the later condition amounts to $P = 0$. ◻

7. Technical results.

Proof of Lemma 10. We monotonically label the vertices of u with the labels $\{1, 2, \ldots, d\}$ and consider the Hamiltonians

$$H^{[\nu]}(y) = \sum_{\substack{i=1,\ldots,d \\ \text{vertex } i \text{ has color } \nu}} q^i \prod_{j \text{ is a son of } i} p^j,$$

with the standard convention that a product over an empty set of indices is 1.

In the corresponding Hamiltonian system, for $i = 1, \ldots, d$,

$$f^{[\mu]i}(y) = -\delta_{\mu\nu_i} \prod_{j \text{ is a son of } i} p^j, \tag{54}$$

where ν_i is the color of vertex i. By setting $i = 1$ in (54), we conclude that, if $F^1(v)(0) \neq 0$, then the root of v must have color ν_1, i.e., the color of the root of u. Furthermore, if the root of u has k sons, then all partial derivatives of

$$\prod_{j \text{ is a son of } 1} p^j$$

of order different from k vanish at the origin. Therefore, $F^1(v)(0) \neq 0$ also implies that in v the root has k sons. We now consider (54) with i a son of the root and apply a similar argument to conclude that, if $F^1(v)(0) \neq 0$, then, in u and v, the sons of the roots are equally colored and have the same number of sons. The iteration of this argument concludes the proof. ∎

Proof of Lemma 6. Given u and v differing only in the color of the root, we label the vertices of u other than the root with the labels $\{3, 4, \dots, d\}$ and construct the Hamiltonian

$$H(y) = p^1 q^2 \prod_{\substack{j \text{ is a son}\\ \text{of the root}}} p^j + \sum_{i=3}^{d} q^i \prod_{j \text{ is a son of } i} p^j.$$

The equations of motion for p^1, p^2, q^1, and q^2 are

$$\begin{aligned}
\dot{p}^1 &= f^1 \equiv 0,\\
\dot{p}^2 &= f^2 = -p^1 \prod_{\substack{j \text{ is a son}\\ \text{of the root}}} p^j,\\
\dot{q}^1 &= f^{d+2} = q^2 \prod_{\substack{j \text{ is a son}\\ \text{of the root}}} p^j,\\
\dot{q}^2 &= f^{d+2} \equiv 0.
\end{aligned}$$

For each ν, we set $f^{[\nu]2} = \delta_{\nu\nu_u} f^2$, where ν_u is the color of the root of u, $f^{[\nu]d+1} = \delta_{\nu\nu_v} f^{d+1}$ and $f^{[\nu]1} = f^{[\nu]d+2} = 0$. This makes $f^{[\nu_u]}$ and $f^{[\nu_v]}$ non-Hamiltonian. The equations of the motion for the variables p^i, $i = 3, \dots, d$, are

$$\dot{p}^i = -\prod_{\substack{j \text{ is a son}\\ \text{of the root}}} p^j$$

and are decomposed as follows (cf. (54)):

$$f^{[\mu]i}(y) = -\delta_{\mu\nu_i} \prod_{j \text{ is a son of } i} p^j. \tag{55}$$

The f^{d+i}, $i = 3, \dots, d$, play no role in the argument and, for simplicity, they are decomposed as $f^{[\nu]d+i} = \delta_{1\nu} f^{d+i}$; i.e., they are all allocated to $f^{[1]}$.

We now prove that for the matrix $F^*(w)$ in Lemma 1, if $w \in \overline{NT}$,

$$F_1^{*k}(w)(0) \neq 0 \Leftrightarrow k = 2, \quad w = u, \tag{56}$$

and

$$F_{d+2}^{*k}(w)(0) \neq 0 \Leftrightarrow k = d+1, \quad w = v. \tag{57}$$

The element $F_1^{*k}(w)(0)$ involves differentiation with respect to p^1. As a consequence, $F_1^{*k}(w)(0)\neq 0$ implies $k=2$, because, for $k\neq 2$, $f^{[\nu]k}$ is either independent of p^1 or depends on p^1 through the combination p^1q^2 and $f^{d+2}\equiv 0$. Then $F_1^{*k}(w)(0)\neq 0$ implies that w is of the form $[w_1,\dots,w_\ell]^{[\nu_u]}$ and

$$F_1^{*k}(w)=\frac{\partial^\ell}{\partial y^{i_1}\partial y^{i_2}\cdots\partial y^{i_\ell}}\frac{\partial f^{[\nu]2}}{\partial p^1}F^{i_1}(w_1)\cdots F^{i_\ell}(w_\ell).$$

By definition of $f^{[\nu]2}$,

$$F_1^{*k}(w)=-\frac{\partial^\ell}{\partial y^{i_1}\partial y^{i_2}\cdots\partial y^{i_\ell}}\left(\prod_{\substack{j\text{ is a son}\\ \text{of the root}}}p^j\right)F^{i_1}(w_1)\cdots F^{i_\ell}(w_\ell).$$

From this formula and (55) we conclude that $w=u$ by using exactly the same argument as in the proof of Lemma 10. Thus (56) holds; (57) is dealt with in a similar way.

Next, by using (32) and induction on the order of w, it is possible to show that (56) and (57) imply, for $w\in\overline{NT}$,

$$F_1^k(w)(0)=F_1^{*k}(w)(0),$$
$$F_{d+2}^k(w)(0)=F_{d+2}^{*k}(w)(0).$$

Now the lemma is a consequence of the formula

$$\left(F'(u)^T(0)JF'(v)(0)\right)_{1,2+d}=\sum_{k=1}^{2d}\pm F_1^k(u)^T(0)F_{2+d}^{\overline{k}}(v)(0),$$

where $\overline{k}$ is the index conjugate to k (i.e. $\overline{k}=k+d$ if $k\leq d$ and $\overline{k}=k-d$ if $k>d$). ☐

Proof of Lemma 5. Given u and v, we label the vertices of u differently from the root with the labels $\{4,\dots,\rho(u)+2\}$ and label the vertices of v differently from the root with labels $\{\rho(u)+3,\dots,d\}$. With each vertex of u or v we associate a "piece" of Hamiltonian function as follows:

$$\text{Root of } u\longrightarrow q^2q^3\prod_{\substack{j\text{ is a son of}\\ \text{the root of } u}}p^j,$$
$$\text{Root of } v\longrightarrow p^1p^3\prod_{\substack{j\text{ is a son of}\\ \text{the root of } v}}p^j,$$
$$\text{Vertex } i\geq 4 \text{ in } u \text{ or } v\longrightarrow q^i\prod_{j\text{ is a son of } i}p^j.$$

Now, for $\nu=1,\dots,N$, $H^{[\nu]}$ is defined by summing the pieces of the vertices of color ν. For instance, if u and v are, respectively, the last and the last but one N-trees in Table 1, the construction above leads to

$$H^{[1]}(y)=q^5+q^6,\qquad H^{[2]}(y)=q^4p^5+p^1p^3p^6p^7+q^7,\qquad H^{[3]}(y)=q^2q^3p^4.$$

To prove that the Hamiltonians $H^{[\nu]}$ constructed here satisfy the conclusion of the lemma we follow an argument similar to that used in the proof of Lemma 6. See also the proof of Lemma 2.2.7 in [17]. ☐

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