SYMPLECTIC GARK METHODS FOR HAMILTONIAN SYSTEMS

MICHAEL GÜNTHER*, ADRIAN SANDU†, AND ANTONELLA ZANNA‡

Abstract. Generalized Additive Runge-Kutta schemes have shown to be a suitable tool for solving ordinary differential equations with additively partitioned right-hand sides. This work generalizes these GARK schemes to symplectic GARK schemes for additively partitioned Hamiltonianm systems. In a general setting, we derive conditions for symplecticeness, as well as symmetry and time-reversibility. We show how symplectic and symmetric schemes can be constructed based on schemes which are only symplectic. Special attention is given to the special case of partitioned schemes for Hamiltonians split into multiple potential and kinetic energies. Finally we show how symplectic GARK schemes can use efficiently different time scales and evaluation costs for different potentials by using different order for these parts.

Key words. Generalized addtive Runge-Kutta methods, Symplectic schemes, symmetric schemes, Partitioned symplectic GARK schemes

AMS subject classifications. 65L05, 65L06, 65L07, 65L020.

1. Introduction. In many applications, initial value problems of ordinary differential equations are given as *additively* partitioned systems

$$y' = f(y) = \sum_{m=1}^{N} f^{\{m\}}(y), \quad y(t_0) = y_0, \tag{1.1}$$

where the right-hand side $f : \mathbb{R}^d \to \mathbb{R}^d$ is split into N different parts with respect to, for example, stiffness, nonlinearity, dynamical behavior, and evaluation cost. Additive partitioning also includes the special case of coordinate partitioning:

$$y' = \begin{bmatrix} y^{\{1\}} \\ \vdots \\ y^{\{N\}} \end{bmatrix}' = \sum_{m=1}^{d} \begin{bmatrix} 0 \\ y^{\{m\}} \\ 0 \end{bmatrix}' = \sum_{m=1}^{d} \begin{bmatrix} 0 \\ f^{\{m\}}(y) \\ 0 \end{bmatrix}. \tag{1.2}$$

One step of a GARK scheme [7] applied to solve (1.1) reads:

$$Y_i^{\{q\}} = y_n + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} \, f^{\{m\}} \left(Y_j^{\{m\}} \right), \tag{1.3a}$$

$$i = 1, \ldots, s^{\{q\}}, \quad q = 1, \ldots, N,$$

$$y_{n+1} = y_n + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \, f^{\{q\}} \left(Y_i^{\{q\}} \right). \tag{1.3b}$$

*Bergische Universität Wuppertal, Institute of Mathematical Modelling, Analysis and Computational Mathematics (IMACM), Gauss strasse 20, D-42119 Wuppertal, Germany (guenther@uni-wuppertal.de)

†Computational Science Laboratory, Department of Computer Science, 2202 Kraft Drive, Virginia Tech, Blacksburg, VA 24060, USA (sandu@cs.vt.edu),

‡Matematisk institutt, Universitetet i Bergen, Norway (Antonella.Zanna@uib.no)

The corresponding generalized Butcher tableau is

$$
\begin{array}{cccc}
\mathbf{A}^{\{1,1\}} & \mathbf{A}^{\{1,2\}} & \dots & \mathbf{A}^{\{1,N\}} \\
\mathbf{A}^{\{2,1\}} & \mathbf{A}^{\{2,2\}} & \dots & \mathbf{A}^{\{2,N\}} \\
\vdots & \vdots & & \vdots \\
\mathbf{A}^{\{N,1\}} & \mathbf{A}^{\{N,2\}} & \dots & \mathbf{A}^{\{N,N\}} \\
\hline
\mathbf{b}^{\{1\}} & \mathbf{b}^{\{2\}} & \dots & \mathbf{b}^{\{N\}}
\end{array}
\tag{1.4}
$$

In contrast to traditional additive methods [4] different stage values are used with different components of the right hand side. The methods $(\mathbf{A}^{\{q,q\}}, \mathbf{b}^{\{q\}})$ can be regarded as stand-alone integration schemes applied to each individual component q. The off-diagonal matrices $\mathbf{A}^{\{q,m\}}$, $m \neq q$, can be viewed as a coupling mechanism among components.

We define the abscissae associated with each tableau as $\mathbf{c}^{\{q,m\}} := \mathbf{A}^{\{q,m\}} \cdot \mathbf{1}^{\{m\}}$. The method (1.4) is *internally consistent* [SG15] if all the abscissae along each row of blocks coincide:

$$\mathbf{c}^{\{q,1\}} = \cdots = \mathbf{c}^{\{q,N\}} =: \mathbf{c}^{\{q\}}, \quad q = 1, \dots, N.$$

Several matrices are defined from the coefficients of (1.3) for $m, \ell = 1, \dots, N$:

$$\mathbf{B}^{\{m\}} = \operatorname{diag}\left(\mathbf{b}^{\{m\}}\right) \in \mathbb{R}^{s^{\{m\}} \times s^{\{m\}}}, \tag{1.5}$$

$$\mathbf{P}^{\{m,\ell\}} = \mathbf{A}^{\{\ell,m\}T}\, \mathbf{B}^{\{\ell\}} + \mathbf{B}^{\{m\}}\, \mathbf{A}^{\{m,\ell\}} - \mathbf{b}^{\{m\}}\, \mathbf{b}^{\{\ell\}T} \in \mathbb{R}^{s^{\{m\}} \times s^{\{\ell\}}}, \tag{1.6}$$

$$\mathbf{P} = [\mathbf{P}^{\{m,\ell\}}]_{1 \le \ell, m \le N} \in \mathbb{R}^{s \times s}, \tag{1.7}$$

where

$$s := \sum_{m=1}^{N} s^{\{m\}}.$$

The condition $\mathbf{P} = \mathbf{0}$ is equivalent to

$$\mathbf{P}^{\{m,\ell\}} := \mathbf{A}^{\{\ell,m\}T}\, \mathbf{B}^{\{\ell\}} + \mathbf{B}^{\{m\}}\, \mathbf{A}^{\{m,\ell\}} - \mathbf{b}^{\{m\}}\, \mathbf{b}^{\{\ell\}T} = 0 \tag{1.8}$$

for all $\ell, m = 1, \dots, N$.

We see that the matrix $\mathbf{P}$ in (1.7) is symmetric since $\mathbf{P}^{\{\ell,m\}} = \mathbf{P}^{\{m,\ell\}T}$. It was shown in [7] that the GARK method is algebraically stable iff the matrix $\mathbf{P}$ is positive definite.

The paper is organized as follows. The next section introduces general symplectic GARK schemes. We derive conditions on the coefficients for symplecticity, which reduce the number of order conditions of GARK schemes drastically, and discuss symmetry and time-reversibility. If the Hamiltonians are split with respect to the potentials or kinetic parts and potentials, resp., partitioned versions of symplectic GARK schemes are tailored to exploit this structure. Section 3 introduces these schemes, with a discussion of symplecticity conditions, order conditions, symmetry and time-reversibility, as well as GARK discrete adjoints. Section 4 discusses how symplectic GARK schemes can exploit the multirate potential given by potentials of different activity levels. Numerical tests for a coupled oscillator are given. Section 5 concludes with a summary.

2. Symplectic GARK schemes — the general case. In this section we consider symplectic systems (1.1) where each partition is a symplectic subsystem in its own right. Specifically, we have $y = (q, p)$ and the Hamiltonian $H(q, p)$ of the total system is the sum of N individual Hamiltonians:

$$H(q,p) = \sum_{\nu=1}^{N} H^{\{\nu\}}(q,p)\,.$$

Each component function corresponds to one individual Hamiltonian,

$$\begin{bmatrix} q' \\ p' \end{bmatrix} = \sum_{\nu=1}^{N} f^{\{\nu\}}(q,p), \qquad f^{\{\nu\}}(q,p) := \begin{bmatrix} \frac{\partial H^{\{\nu\}}(q,p)}{\partial p} \\ -\frac{\partial H^{\{\nu\}}(q,p)}{\partial q} \end{bmatrix}. \tag{2.1}$$

2.1. GARK schemes for partitioned Hamiltonian systems. One step of the GARK method (1.3) applied to (2.1) advances the solution (q_0, p_0) at t_0 to the solution (q_1, p_1) at $t_1 = t_0 + h$ as follows:

$$P_i^{\{q\}} = p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} k_j^{\{m\}}, \tag{2.2a}$$

$$Q_i^{\{q\}} = q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} \ell_j^{\{m\}}, \tag{2.2b}$$

$$p_1 = p_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} k_i^{\{q\}}, \tag{2.2c}$$

$$q_1 = q_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \ell_i^{\{q\}}, \tag{2.2d}$$

$$k_i^{\{m\}} = -\frac{\partial H^{\{m\}}}{\partial q} \left(P_i^{\{m\}}, Q_i^{\{m\}} \right), \tag{2.2e}$$

$$\ell_i^{\{m\}} = \frac{\partial H^{\{m\}}}{\partial p} \left(P_i^{\{m\}}, Q_i^{\{m\}} \right). \tag{2.2f}$$

We have the following property that generalizes the characterization of symplectic Runge Kutta schemes [3].

THEOREM 2.1 (Symplectic GARK schemes). *Consider a GARK scheme* (2.2)*, and its matrix* $\mathbf{P}$ *defined by* (1.7)*. The GARK scheme is symplectic if and only if* $\mathbf{P} = \mathbf{0}$.

Proof. The proof is similar to the proof for Runge-Kutta, partitioned Runge-Kutta methods [9] and ARK schemes [1]. An alternative proof using differential forms is given in the appendix. □

If we split with respect to potentials to exploit their respective behaviour, we get

COROLLARY 2.2. *If a separable Hamiltonian is split into the kinetic part* $T(p)$ *and* $N-1$ *potentials* $U_i(q)$ $(i > 1)$ *with different levels of dynamics and computational costs, i.e.,* $H^{\{1\}} := T(p)$ *and* $H^{\{i\}} := U_i(q)$ $(i > 1)$ *such that*

$$H(q,p) = T(p) + U(q) = T(p) + \sum_{i=2}^{N} U_i(q) = \sum_{i=1}^{N} H^{\{i\}},$$

then the conditions $P^{\{1,1\}} = 0$ *and* $P^{\{\ell,m\}} = 0$ *for* $\ell, m \in \{2, \ldots, N\}$ *are not necessary for the symplecticity of the GARK scheme.*

Proof. This follows directly from the proof in theorem 2.1, as in this case $k_i^{\{1\},J} = 0$ and $\ell_j^{\{m\},J} = 0$ for $m > 1$, which yields (see appendix 5)

$$dk_i^{\{1\},J} \wedge d\ell_j^{\{m\},J} = 0 \quad \text{for } m = 1, \ldots, N,$$
$$dk_i^{\{\ell\},J} \wedge d\ell_j^{\{m\},J} = 0 \quad \text{for } \ell, m = 2, \ldots, N.$$

Hence only the conditions $P^{\{1,m\}} = 0$ for $m > 1$ has to hold, which is equivalent to $P^{\{m,1\}} = 0$ for $m > 1$ due to the symmetry of $\mathbf{P}$. ▯

REMARK 1 (Symplecticity condition and NB series). *The symplectic condition* $\mathbf{P} = 0$ *can be rewritten in terms of NB-series coefficients of the symplectic GARK scheme, as the GARK numerical solutions are NB-series. Let* $u = [u_1, \ldots, u_r]_{\{m\}}$ *and* $v = [v_1, \ldots, v_p]_{\{n\}}$. *The Butcher product of the trees is*

$$u \bullet v := \begin{cases} u, & v = \emptyset, \\ [v]_{\{m\}}, & u = \tau_{\{m\}}, \\ [u_1, \ldots, u_r, v]_{\{m\}}, & \textit{otherwise}. \end{cases}$$

Consider the NB-series associated with a partitioning where each component is Hamiltonian. In Araujo et al, 1997, it is shown that the NB-series $\mathfrak{a}$ *is symplectic iff for each pair of nonempty N-trees it holds that*

$$\mathfrak{a}(u \bullet v) + \mathfrak{a}(v \bullet u) = \mathfrak{a}(u)\,\mathfrak{a}(v). \tag{2.3}$$

For the non-empty NB-trees u and v above we get

$$a(u) = \mathbf{b}^{\{m,\top\}} U = \sum_{i=1}^{s^{\{m\}}} b_i^{\{m\}} U_i,$$
$$a(v) = \mathbf{b}^{\{n,\top\}} V = \sum_{j=1}^{s^{\{n\}}} b_j^{\{n\}} V_j,$$
$$a(u \bullet v) = \mathbf{b}^{\{m,\top\}} \left(U \times \mathbf{A}^{\{m,n\}} V \right) = \sum_{i=1}^{s^{\{m\}}} \sum_{j=1}^{s^{\{n\}}} b_i^{\{m\}} U_i \mathbf{A}_{i,j}^{\{m,n\}} V_j,$$
$$a(v \bullet u) = \mathbf{b}^{\{n,\top\}} \left(V \times \mathbf{A}^{\{n,m\}} U \right) = \sum_{j=1}^{s^{\{n\}}} \sum_{i=1}^{s^{\{m\}}} b_j^{\{n\}} V_j \mathbf{A}_{j,i}^{\{n,m\}} U_i,$$

where we have used the abbreviations

$$U := a(u_1) \times \cdots \times a(u_r), \quad V := a(v_1) \times \cdots \times a(u_p).$$

From (2.3) *we get after reordering the coefficients*

$$\sum_{i=1}^{s^{\{m\}}} \sum_{j=1}^{s^{\{n\}}} \left(b_i^{\{m\}} \mathbf{A}_{i,j}^{\{m,n\}} + b_j^{\{n\}} {\mathbf{A}^{\top}}_{i,j}^{\{n,m\}} - b_i^{\{m,\top\}} b_j^{\{n\}} \right) U_i V_j = 0,$$

which is equivalent to $\mathbf{P} = \mathbf{0}$.

2.2. Order conditions. As shown in [7], the order conditions for a GARK method (1.3) are obtained from the order conditions of ordinary Runge–Kutta methods. The usual labeling of the Runge-Kutta coefficients (subscripts $i, j, k, \ldots$) is accompanied by a corresponding labeling of the different partitions for the N-tree (superscripts $\sigma, \nu, \mu, \ldots$).

Let $\mathbf{1}^{\{\nu\}}$ be a vector of ones of dimension $s^{\{\nu\}}$, and $\mathbf{c}^{\{\sigma,\nu\}} := \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{1}^{\{\nu\}}$. The specific conditions for orders one to four are as follows.

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{1}^{\{\sigma\}} = 1, \quad \forall\, \sigma. \qquad \text{(order 1)} \tag{2.4a}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{c}^{\{\sigma,\nu\}} = \frac{1}{2}, \quad \forall\, \sigma, \nu, \qquad \text{(order 2)} \tag{2.4b}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma,\nu\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right) = \frac{1}{3}, \quad \forall\, \sigma, \nu, \mu, \qquad \text{(order 3)} \tag{2.4c}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu,\mu\}} = \frac{1}{6}, \quad \forall\, \sigma, \nu, \mu, \qquad \text{(order 3)} \tag{2.4d}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma,\nu\}} \times \mathbf{c}^{\{\sigma,\lambda\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right) = \frac{1}{4}, \quad \forall\, \sigma, \nu, \lambda, \mu, \qquad \text{(order 4)} \tag{2.4e}$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right)^{\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu,\lambda\}} = \frac{1}{8}, \quad \forall\, \sigma, \nu, \lambda, \mu, \qquad \text{(order 4)} \tag{2.4f}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \left(\mathbf{c}^{\{\nu,\lambda\}} \times \mathbf{c}^{\{\nu,\mu\}}\right) = \frac{1}{12}, \quad \forall\, \sigma, \nu, \lambda, \mu, \qquad \text{(order 4)} \tag{2.4g}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{A}^{\{\nu,\lambda\}} \cdot \mathbf{c}^{\{\lambda,\mu\}} = \frac{1}{24}, \quad \forall\, \sigma, \nu, \lambda, \mu. \qquad \text{(order 4)} \tag{2.4h}$$

Here, the standard matrix and vector multiplication is denoted by dot (e.g., $\mathbf{b}^T \cdot \mathbf{c}$ is a dot product), whereas the cross denotes component-wise multiplication (e.g., $\mathbf{b} \times \mathbf{c}$ is a vector of element-wise products).

For internally consistent schemes these order conditions simplify to

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{1}^{\{\sigma\}} = 1, \quad \forall\, \sigma. \qquad \text{(order 1)} \tag{2.5a}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{c}^{\{\sigma\}} = \frac{1}{2}, \quad \forall\, \sigma, \qquad \text{(order 2)} \tag{2.5b}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}}\right) = \frac{1}{3}, \quad \forall\, \sigma, \qquad \text{(order 3)} \tag{2.5c}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu\}} = \frac{1}{6}, \quad \forall\, \sigma, \nu, \qquad \text{(order 3)} \tag{2.5d}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}}\right) = \frac{1}{4}, \quad \forall\, \sigma \qquad \text{(order 4)} \tag{2.5e}$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma\}}\right)^{\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu\}} = \frac{1}{8}, \quad \forall\, \sigma, \nu, \qquad \text{(order 4)} \tag{2.5f}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \left(\mathbf{c}^{\{\nu\}} \times \mathbf{c}^{\{\nu\}}\right) = \frac{1}{12}, \quad \forall\, \sigma, \nu, \qquad \text{(order 4)} \tag{2.5g}$$

$$\mathbf{b}^{\{\sigma\}\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \mathbf{A}^{\{\nu,\lambda\}} \cdot \mathbf{c}^{\{\lambda\}} = \frac{1}{24}, \quad \forall\, \sigma, \nu, \lambda. \qquad \text{(order 4)} \tag{2.5h}$$

For symplectic GARK schemes, the order conditions above are redundant, as we have

Remark 2 (Redundancy of order conditions for symplectic GARK schemes). *Assume that the symplectic GARK method with NB series coefficients $\mathfrak{c}(u)$ satisfies all conditions up to order k, i.e.,*

$$\mathfrak{c}(u) = 1/\gamma(u) \quad \forall c: \ \rho(u) \le k.$$

If the order is $k+1$, then (2.3) *implies*

$$\mathfrak{c}(u \bullet v) + \mathfrak{c}(v \bullet u) = \frac{1}{\gamma(u)} \frac{1}{\gamma(v)}. \tag{2.6}$$

This defines the following relations for order conditions:

- *For* $v = \tau_{\{l\}}$ *and* $u = [u_1, \ldots, u_r]_{\{m\}}$ *we have*

$$u \bullet v = [u_1, \ldots, u_r, \tau_{\{\ell\}}]_{\{m\}}, \quad v \bullet u = [[u_1, \ldots, u_r]_{\{m\}}]_{\{\ell\}},$$

  and thus (2.6) *yields*

$$c([u_1, \ldots, u_r, \tau_{\{\ell\}}]_{\{m\}}) + c([[u_1, \ldots, u_r]_{\{m\}}]_{\{\ell\}}) = c(\tau_{\{l\}})c([u_1, \ldots, u_r]_{\{m\}}),$$

  which implies the order $k+1$ *relation*

$$\mathbf{b}^{\{m\}T} (U \times \mathbf{c}^{\{m,\ell\}}) + \mathbf{b}^{\{\ell\}T} \mathbf{A}^{\{\ell,m\}} U = \frac{1}{\gamma([u_1, \ldots, u_r]_{\{m\}})}, \tag{2.7}$$

  where $U =_{i=1}^{r} a(u_i)$.

- *For* $v = [\tau_{\{s\}}]_{\{l\}}$ *and* $u = [\tau_{\{t\}}]_{\{m\}}$ *we have*

$$u \bullet v = [\tau_{\{t\}}, [\tau_{\{s\}}]_{\{l\}}]_{\{m\}},$$
$$v \bullet u = [\tau_{\{s\}}, [\tau_{\{t\}}]_{\{m\}}]_{\{l\}},$$

  and thus (2.6) *leads to*

$$c([\tau_{\{t\}}, [\tau_{\{s\}}]_{\{l\}}]_{\{m\}}) + c([\tau_{\{s\}}, [\tau_{\{t\}}]_{\{m\}}]_{\{l\}}) = c([\tau_{\{t\}}]_{\{m\}})c([\tau_{\{s\}}]_{\{l\}}),$$

  which implies the order four relation

$$\begin{aligned} &\mathbf{b}^{\{m\}T} (\mathbf{c}^{\{m,t\}} \times \mathbf{A}^{\{m,l\}} \mathbf{c}^{\{l,s\}}) + \\ &\quad \mathbf{b}^{\{\ell\}T} (\mathbf{c}^{\{l,s\}} \times \mathbf{A}^{\{l,m\}} \mathbf{c}^{\{m,t\}}) = \frac{1}{\gamma([\tau_{\{t\}}]_{\{m\}})} \frac{1}{\gamma([\tau_{\{s\}}]_{\{l\}})} = \frac{1}{4}. \end{aligned} \tag{2.8}$$

Thus we get

THEOREM 2.3. *For symplectic GARK schemes the number of order conditions is reduced due to redundancy:*

- *order 2: the number of* N^2 *order conditions reduces to only* $\mathrm{N}(\mathrm{N}-1)/2$ *order conditions;*
- *order 3: the number of* $2\mathrm{N}^3$ *order conditions reduces to only* N^3 *order conditions, if the scheme is of order 2 at least;*
- *order 4: the number of* $4\mathrm{N}^4$ *order conditions reduces to only* $\mathrm{N}^2(3\mathrm{N}^2-1)/2$ *order conditions, if the scheme is of order 3 at least;*

If the scheme is internally consistent, then

- *order 2: the order two condition* (2.5b) *is automatically fulfilled;*
- *order 3: if the scheme has order two at least, only the* N *order conditions* (2.5c) *have to be fulfilled;*
- *order 4: if the scheme has order three at least, then only the order four conditions* (2.5f) *for* $\sigma < \nu$ *and* (2.5e) *have to be fulfilled.*

Proof. We assume that the symplectic GARK scheme has order one at least. *Order two.* Using the redundancy relation (2.7) with $u = \tau_{\{m\}}$, we get

$$\mathbf{b}^{\{m\}T} \mathbf{c}^{\{m,\ell\}}) + \mathbf{b}^{\{\ell\}T} \mathbf{c}^{\{\ell,m\}} - 1 = 0, \tag{2.9}$$

which yields for $\ell = m$ the order two conditions

$$\mathbf{b}^{\{m\}\top}\mathbf{c}^{\{m,m\}} = \frac{1}{2};$$

Assuming that the order two condition

$$\mathbf{b}^{\{m\}\top}\mathbf{c}^{\{m,\ell\}} = \frac{1}{2}$$

holds for $\ell < m$, (2.9) yields the order two condition for $\ell > m$.

Order three. Using the redundancy relation (2.7) with $u = [\tau_{\{s\}}]_{\{m\}}$, we get

$$\mathbf{b}^{\{m\}T}\left(\mathbf{c}^{\{m,s\}} \times \mathbf{c}^{\{m,\ell\}}\right) + \mathbf{b}^{\{\ell\}T}\,\mathbf{A}^{\{\ell,m\}}\,\mathbf{c}^{\{m,s\}} = \frac{1}{2}.$$

Thus the order three condition

$$\mathbf{b}^{\{\ell\}\top}(\mathbf{c}^{\{\ell,m\}} \times \mathbf{c}^{\{\ell,s\}}) = \frac{1}{3} \qquad (2.10)$$

yields the order condition

$$\mathbf{b}^{\{m\}\top}\mathbf{A}^{\{m,\ell\}}\mathbf{c}^{\{\ell,s\}} = \frac{1}{6}$$

and vice versa.

Order four. Using the redundancy relation (2.7) with $u = [[\tau_{\{l\}}]_{\{s\}}]_{\{m\}}$, we get

$$\mathbf{b}^{\{m\}T}\left(\mathbf{A}^{\{m,s\}}\,\mathbf{c}^{\{s,l\}} \times \mathbf{c}^{\{m,t\}}\right) + \mathbf{b}^{\{t\}T}\,\mathbf{A}^{\{t,m\}}\,\mathbf{A}^{\{m,s\}}\,\mathbf{c}^{\{s,l\}} - \frac{1}{6} = 0. \qquad (2.11)$$

Using the redundancy relation (2.7) with $u = [\tau_{\{s\}}, \tau_{\{t\}}]_{\{l\}}$, we get

$$\mathbf{b}^{\{l\}T}\left(\mathbf{c}^{\{l,s\}} \times \mathbf{c}^{\{l,t\}}\right) \times \mathbf{c}^{\{l,m\}}) + \mathbf{b}^{\{m\}T}\,\mathbf{A}^{\{m,l\}}\left(\mathbf{c}^{\{l,s\}} \times \mathbf{c}^{\{l,t\}}\right) - \frac{1}{3} = 0. \qquad (2.12)$$

Setting $t = l$ and $m = s$, the second redundancy relation (2.8) yields the N^2 order four conditions

$$\mathbf{b}^{\{\ell\}T}\left(\mathbf{c}^{\{l,t\}} \times \mathbf{A}^{\{l,l\}}\,\mathbf{c}^{\{l,t\}}\right) - \frac{1}{8} = 0$$

as part of (2.4f). If in addition

$$\mathbf{b}^{\{\ell\}T}\left(\mathbf{c}^{\{l,m\}} \times \mathbf{A}^{\{l,t\}}\,\mathbf{c}^{\{t,s\}}\right) - \frac{1}{8} = 0$$

holds for $\ell + m \le t + s$, then the overall $\mathrm{N}^2(\mathrm{N}^2-1)/2$ conditions are equivalent to (2.4f). Assuming now that these $\mathrm{N}^2(\mathrm{N}^2-1)/2$ conditions hold, (2.11) yields the N^4 order conditions (2.4h). Finally, (2.12) yields (2.4e), if (2.4g) holds, and vice versa.

The proposition for internally consistent schemes follows directly from the results above.

Order two. From (2.9) we get the N order two conditions (2.5b).

Order three. Here the order conditions (2.10) reduce to the N order conditions (2.5c)..

Order four. If the $\mathrm{N}(\mathrm{N}-1)/2$ order conditions

$$(\mathbf{b}^{\{\ell\}} \times \mathbf{c}^{\{\ell\}})^{\mathrm{T}}\mathbf{A}^{\{\ell,t\}}\mathbf{c}^{\{t\}}) = \frac{1}{8}.$$

for $\ell < t$ hold, then the N^2 order conditions (2.5f) are fulfilled, and as before the N^4 order conditions (2.5h). Assuming now that the N order conditions of (2.5e) are fulfilled, the N^2 order conditions (2.4g) hold. □

2.3. Symmetry and time-reversibility. REMARK 3 (Time-reversed GARK method). *Let $\mathcal{P} \in \mathbb{R}^{s\times s}$ be the permutation matrix that reverses the entries of a vector. In matrix notation the time-reversed GARK method is:*

$$\underline{\mathbf{b}}^{\{m\}} := \mathcal{P}\,\mathbf{b}^{\{m\}} \quad \Leftrightarrow \quad \underline{b}_j^{\{m\}} = b_{s+1-j}^{\{m\}}, \quad \forall j; \tag{2.13a}$$

$$\begin{aligned}\underline{\mathbf{A}}^{\{\ell,m\}} &:= \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} \\ &\Leftrightarrow \quad \underline{a}_{i,j}^{\{\ell,m\}} = b_j^{\{m\}} - a_{s^{\{\ell\}}+1-i,s^{\{m\}}+1-j}^{\{\ell,m\}}, \quad \forall i,j.\end{aligned} \tag{2.13b}$$

DEFINITION 2.4 (Symmetric GARK schemes). *The GARK scheme* (2.2) *is symmetric if it is invariant with respect to time reversion* (2.13)*:*

$$\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}} \quad \Leftrightarrow \quad b_j^{\{m\}} = b_{s+1-j}^{\{m\}}, \quad \forall j; \tag{2.14a}$$

$$\mathbf{A}^{\{\ell,m\}} = \underline{\mathbf{A}}^{\{\ell,m\}} \quad \Leftrightarrow \quad a_{i,j}^{\{\ell,m\}} = b_j^{\{m\}} - a_{s^{\{\ell\}}+1-i,s^{\{m\}}+1-j}^{\{\ell,m\}}, \quad \forall i,j. \tag{2.14b}$$

Note that (2.14b) implies (2.14a). From (2.13b) and (2.14b)

$$\mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} + \mathbf{A}^{\{\ell,m\}} = \mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} + \underline{\mathbf{A}}^{\{\ell,m\}} = \mathbf{1}\,\mathbf{b}^{\{m\}T},$$

and multiplying this equation from left and right with $\mathcal{P}$ yields

$$\mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} + \mathbf{A}^{\{\ell,m\}} = \mathbf{1}\,\mathbf{b}^{\{m\}T}\,\mathcal{P},$$

which implies $\mathcal{P}\,\mathbf{b}^{\{m\}} = \mathbf{b}^{\{m\}}$.

REMARK 4 (Symplecticness of time-reversed GARK methods). *Consider the case where the base method is symplectic* (1.8) . *The symplecticness condition* (1.8) *for the time-reversed scheme* (2.13) *reads:*

$$\begin{aligned}
&\underline{\mathbf{A}}^{\{\ell,m\}T}\,\underline{\mathbf{B}}^{\{\ell\}} + \underline{\mathbf{b}}^{\{m\}}\,\underline{\mathbf{A}}^{\{m,\ell\}} - \underline{\mathbf{b}}^{\{m\}}\,\underline{\mathbf{b}}^{\{\ell\}T} \\
=& \left(\mathbf{b}^{\{m\}}\,\mathbf{1}^T - \mathcal{P}\,\mathbf{A}^{\{\ell,m\}T}\,\mathcal{P}\right)\left(\mathcal{P}\,\mathbf{b}^{\{\ell\}}\mathcal{P}\right) \\
&\quad + \left(\mathcal{P}\,\mathbf{b}^{\{m\}}\mathcal{P}\right)\left(\mathbf{1}\,\mathbf{b}^{\{\ell\}T} - \mathcal{P}\,\mathbf{A}^{\{m,\ell\}}\,\mathcal{P}\right) - \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\mathcal{P} \\
=& \mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\,\mathcal{P} - \mathcal{P}\left(\mathbf{A}^{\{\ell,m\}T}\,\mathbf{b}^{\{\ell\}} + \mathbf{b}^{\{m\}}\,\mathbf{A}^{\{m,\ell\}}\right)\mathcal{P} \\
&\quad + \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T} - \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\mathcal{P} \\
=& \mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\,\mathcal{P} - \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\,\mathcal{P} \\
&\quad + \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T} - \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\mathcal{P}
\end{aligned}$$

and therefore

$$\begin{aligned}
&\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\,\mathcal{P} + \mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T} = 2\,\mathcal{P}\,\mathbf{b}^{\{m\}}\,\mathbf{b}^{\{\ell\}T}\mathcal{P} \\
\Leftrightarrow \quad &\left(\mathbf{b}_i^{\{m\}} - \mathbf{b}_{s^{\{m\}}+1-i}^{\{m\}}\right)\mathbf{b}_{s^{\{\ell\}}+1-j}^{\{\ell\}} + \mathbf{b}_{s^{\{m\}}+1-i}^{\{m\}}\left(\mathbf{b}_j^{\{\ell\}} - \mathbf{b}_{s^{\{\ell\}}+1-j}^{\{\ell\}}\right) = 0, \quad \forall i,j.
\end{aligned}$$

A sufficient condition for symplecticness of the time-reversed scheme is:

$$\mathbf{b}^{\{m\}} = \mathcal{P}\,\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}, \qquad \mathbf{b}^{\{\ell\}} = \mathcal{P}\,\mathbf{b}^{\{\ell\}} = \underline{\mathbf{b}}^{\{\ell\}}.$$

With the help of time-reversed symplectic GARK methods one can derive symmetric and symplectic GARK methods:

THEOREM 2.5. *Assume that the GARK scheme* $\left(\mathbf{A}^{\{\ell,m\}}, b^{\{m\}}\right)$ *is symplectic. If* $b^{\{m\}} = \mathcal{P} b^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}$ *holds, the GARK scheme defined by applying one step with the GARK scheme, followed by one step with its time-reversed GARK scheme, i.e.,*

$$\left(\begin{bmatrix} \mathbf{A}^{\{\ell,m\}} & 0 \\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{\ell,m\}} \end{bmatrix}, \begin{bmatrix} \mathbf{b}^{\{m\}} \\ \underline{\mathbf{b}}^{\{m\}} \end{bmatrix} \right) \tag{2.15}$$

is both symmetric and symplectic.

Proof. For symmetry we have to show, using $\underline{\mathbf{b}}^{\{m\}} = \mathbf{b}^{\{m\}}$,

$$\begin{pmatrix} \mathbf{A}^{\{\ell,m\}} & 0 \\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{\ell,m\}} \end{pmatrix} + \begin{pmatrix} 0 & \mathcal{P} \\ \mathcal{P} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{A}^{\{\ell,m\}} & 0 \\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{\ell,m\}} \end{pmatrix} \begin{pmatrix} 0 & \mathcal{P} \\ \mathcal{P} & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{1}\mathbf{b}^{\{m\}T} & \mathbf{1}\mathbf{b}^{\{m\}T} \\ \mathbf{1}\mathbf{b}^{\{m\}T} & \mathbf{1}\mathbf{b}^{\{m\}T} \end{pmatrix},$$

which is equivalent to $\mathcal{P}\mathbf{b}^{\{m\}} = \mathbf{b}^{\{m\}}$. Symplecticeness requires

$$\begin{pmatrix} \mathbf{A}^{\{\ell,m\}} & 0 \\ \mathbf{1}\mathbf{b}^{\{m\}} & \underline{\mathbf{A}}^{\{\ell,m\}} \end{pmatrix} = \begin{pmatrix} \mathbf{1}\mathbf{b}^{\{m\}} & \mathbf{1}\mathbf{b}^{\{m\}} \\ \mathbf{1}\mathbf{b}^{\{m\}} & \mathbf{1}\mathbf{b}^{\{m\}} \end{pmatrix} - \begin{pmatrix} \mathbf{B}^{\{\ell\}-1} & 0 \\ 0 & \mathbf{B}^{\{\ell\}-1} \end{pmatrix} \begin{pmatrix} \mathbf{A}^{\{m,l\}T} & \mathbf{b}^{\{\ell\}}\mathbf{1}^T \\ 0 & \underline{\mathbf{A}}^{\{m,l\}T} \end{pmatrix} \begin{pmatrix} \mathbf{B}^{\{m\}} & 0 \\ 0 & \mathbf{B}^{\{m\}} \end{pmatrix},$$

which holds for a symplectic partitioned scheme $\left(\mathbf{A}^{\{\ell,m\}}, \mathbf{b}^{\{m\}}\right)$. □

REMARK 5. *One drawback of this construction is the low degree of freedom* $\lceil s^{\{m\}}/2 \rceil$ *in the weights* $\mathbf{b}^{\{m\}}$.

Symplecticness condition (for $\mathbf{b}_i^{\{\ell\}} \neq 0$) plus symmetry requires in the general case that:

$$\begin{aligned} 0 &= \mathbf{b}^{\{\ell\}-1}\, \mathbf{A}^{\{m,\ell\}T}\, \mathbf{b}^{\{m\}} + \mathbf{A}^{\{\ell,m\}} - \mathbf{1}\, \mathbf{b}^{\{m\}T} \\ &= \mathbf{b}^{\{\ell\}-1}\, \mathbf{A}^{\{m,\ell\}T}\, \mathbf{b}^{\{m\}} - \mathcal{P}\, \mathbf{A}^{\{\ell,m\}}\, \mathcal{P} \\ \mathbf{A}^{\{m,\ell\}T}\, \mathbf{b}^{\{m\}} &= \mathbf{b}^{\{\ell\}}\, (\mathcal{P}\, \mathbf{A}^{\{\ell,m\}}\, \mathcal{P}) \\ b_j^{\{m\}}\, a_{j,i}^{\{m,\ell\}} &= b_i^{\{\ell\}}\, a_{s+1-i,s+1-j}^{\{\ell,m\}}. \end{aligned} \tag{2.16}$$

This condition, together with symmetry implies symplecticness, and vice versa, together with symplecticness it implies symmetry.

$$\{\textit{symmetric}\} \cap \{\textit{symplectic}\} \quad \Leftrightarrow \quad \textit{symmetric} \cap (2.16) \quad \Leftrightarrow \quad (2.16) \cap \textit{symplectic}.$$

REMARK 6. *The condition* (2.16) *is only necessary for symplecticness and symmetry, but not sufficient for either symplecticness or symmetry, as the following counterexample for* $N = 1$ *and two stages shows. Condition* (2.16) *reads in this case*

$$a_{2,2} = a_{1,1} \quad \text{and} \quad b_1 = b_2 \tag{2.17}$$

Symmetry requires that

$$\begin{pmatrix} a_{2,2} & a_{2,1} \\ a_{1,2} & a_{1,1} \end{pmatrix} + \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} = \begin{pmatrix} b_1 & b_2 \\ b_1 & b_2 \end{pmatrix},$$

holds, which yields the conditions

$$
\begin{aligned}
b_1 &= b_2, \\
a_{1,1} + a_{2,2} &= b_1, \\
a_{1,2} + a_{2,1} &= b_1.
\end{aligned}
\tag{2.18}
$$

Symplecticness is given, if

$$
\begin{pmatrix} \frac{1}{b_1} & 0 \\ 0 & \frac{1}{b_2} \end{pmatrix} \begin{pmatrix} a_{1,1} & a_{2,1} \\ a_{1,2} & a_{2,2} \end{pmatrix} \begin{pmatrix} b_1 & 0 \\ 0 & b_2 \end{pmatrix} + \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} - \begin{pmatrix} b_1 & b_2 \\ b_1 & b_2 \end{pmatrix} = 0,
$$

holds, which yields the conditions

$$
\begin{aligned}
a_{1,1} &= \frac{b_1}{2}, \\
a_{2,2} &= \frac{b_2}{2}, \\
a_{1,2}b_1 + a_{2,1}b_2 &= b_1 b_2.
\end{aligned}
\tag{2.19}
$$

Clearly, condition (2.17) *neither implies* (2.18) *nor* (2.19).

When dealing with Hamiltonian systems, time-reversibility of a scheme is a desirable property. Introducing the linear mapping given by the regular matrix

$$
\rho = \begin{bmatrix} \mathbf{I}_{d_q \times d_q} & \mathbf{0}_{d_q \times d_p} \\ \mathbf{0}_{d_p \times d_q} & -\mathbf{I}_{d_p \times d_p} \end{bmatrix},
$$

time reversibility of a one step scheme φ_h is defined as the property that

$$
\rho \circ \varphi_h \circ \rho \circ \varphi_h = \mathbf{I},
$$

i.e., the mapping defined by first applying one step with step size h, then changing the sign of the momentum p only, applying a second step with step size h, and finally changing the sign of p again is the identity mapping. If the scheme is symmetric time reversibility is equivalent to the condition [3].

$$
\rho \circ \varphi_h = \varphi_{-h} \circ \rho,
\tag{2.20}
$$

In the following we will show that the symmetry of a GARK scheme is sufficient for being time-reversible.

THEOREM 2.6 (Symmetric GARK schemes are time-reversible). *If the GARK scheme* (2.2) *is symmetric then it is time-reversible, provided that the partitions are Hamiltonian.*

Proof. Apply the GARK step (2.2) to the initial values $\rho(q_0, p_0) = (q_0, -p_0)$ with step size $-h$ to obtain

$$
\begin{aligned}
P_i^{\{q\}} &= (-p_0) + (-h) \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} k_j^{\{m\}},\\
Q_i^{\{q\}} &= q_0 + (-h) \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} \ell_j^{\{m\}},\\
p_1 &= (-p_0) + (-h) \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} k_i^{\{q\}},\\
q_1 &= q_0 + (-h) \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \ell_i^{\{q\}}.
\end{aligned}
$$

As the partitions are Hamiltonian and therefore time-reversible

$$
\begin{aligned}
k_i^{\{m\}} &= -\frac{\partial H^{\{m\}}}{\partial q}(P_i^{\{m\}}, Q_i^{\{m\}}) = -\frac{\partial H^{\{m\}}}{\partial q}(-P_i^{\{m\}}, Q_i^{\{m\}}),\\
\ell_i^{\{m\}} &= \frac{\partial H^{\{m\}}}{\partial p}(P_i^{\{m\}}, Q_i^{\{m\}}) = -\frac{\partial H^{\{m\}}}{\partial p}(-P_i^{\{m\}}, Q_i^{\{m\}}).
\end{aligned}
$$

Renaming the variables $P_i^{\{m\}} := -P_i^{\{m\}}$ and $k_i^{\{m\}} := -k_i^{\{m\}}$ leads to the scheme

$$
\begin{aligned}
P_i^{\{q\}} &= p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} k_j^{\{m\}},\\
Q_i^{\{q\}} &= q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} \ell_j^{\{m\}},\\
p_1 &= -\left(p_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} k_i^{\{q\}} \right),\\
q_1 &= q_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \ell_i^{\{q\}},
\end{aligned}
$$

which immediately shows that (2.20) holds for the GARK scheme. □

The proof may be generalized to the setting of ρ-reversibility with $\rho(q,p) = (\rho_1(q), \rho_2(p))$.

EXAMPLE 1 (A symplectic implicit-implicit scheme). *Consider the GARK scheme* (2.2) *defined by the generalized Butcher tableau* (1.4)

$$
\begin{array}{c|c}
\mathbf{A}^{\{1,1\}} & \mathbf{A}^{\{1,2\}} \\ \hline
\mathbf{A}^{\{2,1\}} & \mathbf{A}^{\{2,2\}} \\ \hline
\mathbf{b}^{\{1\}} & \mathbf{b}^{\{2\}}
\end{array}
:=
\begin{array}{cc|cc}
\frac{1}{8} & 0 & 0 & 0 \\
\frac{1}{4} & \frac{3}{8} & \frac{2}{3} & 0 \\ \hline
\frac{1}{4} & 0 & \frac{1}{3} & 0 \\
\frac{1}{4} & \frac{3}{4} & \frac{2}{3} & \frac{1}{6} \\ \hline
\frac{1}{4} & \frac{3}{4} & \frac{2}{3} & \frac{1}{3}
\end{array}.
$$

This scheme is symplectic according to Theorem 2.1. However, the scheme is not symmetric.

EXAMPLE 2 (A symplectic and symmetric implicit-implicit GARK).

A symmetric and symplectic GARK method of order two, based on the Verlet scheme in the coupling parts, is characterized by the generalized Butcher tableau (1.4)

$$
\begin{array}{cc|cc}
\frac{1}{4} & \alpha & 0 & 0 \\
\frac{1}{2}-\alpha & \frac{1}{4} & \frac{1}{2} & \frac{1}{2} \\
\hline
\frac{1}{2} & 0 & \frac{1}{4} & \beta \\
\frac{1}{2} & 0 & \frac{1}{2}-\beta & \frac{1}{4} \\
\hline
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

where α, β are free real parameters. One notes that this scheme, if applied to a separable Hamiltonian system in a coordinate partitioning way, is equivalent to the Verlet scheme.

3. Partitioned GARK schemes for separable Hamiltonian systems. In the following we discuss two different types of partitioned Hamiltonians in the case of separable Hamiltonians $H(q,p) = T(p) + V(q)$, for which we will derive partitioned symplectic GARK schemes:

- Splitting of the potential:

$$
\begin{aligned}
H(q,p) &= \sum_{i=1}^{N} H^{\{i\}}(q,p), \quad \text{with} \\
H^{\{1\}}(q,p) &= T(p), \\
H^{\{i\}}(q,p) &= V^{\{i\}}(q), \quad i = 2,\dots,N, \\
V(q) &= \sum_{i=2}^{N} V^{\{i\}}(q)
\end{aligned}
$$

- Splitting of both kinitic part and potenial:

$$
\begin{aligned}
H(q,p) &= \sum_{i=1}^{2N} H^{\{i\}}(q,p), \quad \text{with} \\
H^{\{i\}}(q,p) &= T^{\{i\}}(p), \quad i = 1,\dots,N, \\
H^{\{i+N\}}(q,p) &= V^{\{i\}}(q), \quad i = 1,\dots,N, \\
T(p) &= \sum_{i=1}^{N} V^{\{i\}}(p), \\
V(q) &= \sum_{i=1}^{N} V^{\{i\}}(q),
\end{aligned}
$$

3.1. Partitioned GARK schemes for potential splitting. The GARK scheme applied to the potential splitting reads

$$
\begin{aligned}
P_i^{\{1\}} &= p_0 - h \sum_{m=2}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{1,m\}} \cdot V'(Q_i^{\{m\}}),\\
Q_i^{\{q\}} &= q_0 + h \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,1\}} \cdot T'(P_i^{\{1\}}), \quad q = 2, \dots, N\\
p_1 &= p_0 - h \sum_{m=2}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{m\}} \cdot V'(Q_i^{\{m\}}),\\
q_1 &= q_0 + h \sum_{i=1}^{s^{\{q\}}} b_i^{\{1\}} \cdot T'(P_i^{\{1\}}).
\end{aligned}
$$

One notes that the computation of the stage vectors $P_i^{\{q\}}$ for $q = 2, \dots, N$ and and $Q_i^{\{1\}}$ is not needed for this type of splitting. Due to corollary 2.2 the symplicticity condition reads

$$
\mathbf{P}^{(1,m)} = \mathbf{A}^{\{m,1\}T}\,\mathbf{B}^{\{m\}} + \mathbf{B}^{\{1\}}\,\mathbf{A}^{\{1,m\}} - \mathbf{b}^{\{1\}}\,\mathbf{b}^{\{m\}T} = 0, \qquad m = 2, \dots, N,
$$

which can be solved for $\mathbf{A}^{\{1,m\}}$:

$$
\mathbf{A}^{\{1,m\}} = \mathbb{1}\,\mathbf{b}^{\{m\}T} - \left(\mathbf{B}^{\{1\}}\right)^{-1} \mathbf{A}^{\{m,1\}T}\mathbf{B}^{\{m\}}. \tag{3.1}
$$

If the $N-1$ Runge Kutta schemes $(\mathbf{b}^{\{2\}}, \mathbf{A}^{\{2,1\}}), \dots, \mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,1\}})$ and $\mathbf{b}^{\{1\}}$ are given, $\mathbf{A}^{\{1,m\}}$ is uniquely defined by (3.1) in the symplectic case. Defining now

$$
\hat{\mathbf{A}}^{\{1,m\}} := \mathbb{1}\,\mathbf{b}^{\{m\}T} - \left(\mathbf{B}^{\{1\}}\right)^{-1} \mathbf{A}^{\{m,1\}T}\mathbf{B}^{\{m\}},
$$

the GARK scheme reads

$$
P_i^{\{1\}} = p_0 - h \sum_{m=2}^{N} \sum_{j=1}^{s^{\{m\}}} \hat{a}_{i,j}^{\{1,m\}} \cdot V'(Q_i^{\{m\}}), \tag{3.2a}
$$

$$
Q_i^{\{q\}} = q_0 + h \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,1\}} \cdot T'(P_i^{\{1\}}), \quad q = 2, \dots, N \tag{3.2b}
$$

$$
p_1 = p_0 - h \sum_{m=2}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{m\}} \cdot V'(Q_i^{\{m\}}), \tag{3.2c}
$$

$$
q_1 = q_0 + h \sum_{i=1}^{s^{\{q\}}} b_i^{\{1\}} \cdot T'(P_i^{\{1\}}). \tag{3.2d}
$$

Remark 7. *For $N = 2$ the scheme is equivalent to a Partitioned RK scheme with Butcher tableau*

$$
\begin{array}{cc}
\mathbf{A} & \hat{\mathbf{A}} \\
\hline
\mathbf{b}^T & \hat{\mathbf{b}}^T
\end{array} \tag{3.3}
$$

with

$$\begin{aligned}
\mathbf{A} &:= \mathbf{A}^{\{2,1\}}, \\
\hat{\mathbf{A}} &:= \hat{\mathbf{A}}^{\{1,2\}} = \mathbb{1}\,\hat{\mathbf{b}}^{\top} - \mathbf{B}^{-1}\mathbf{A}^{\{2,1\}T}\hat{\mathbf{B}}, \\
\mathbf{b} &:= \mathbf{b}^{\{1\}}, \\
\hat{\mathbf{b}} &:= \mathbf{b}^{\{2\}}.
\end{aligned}$$

The choice of $N-1$ *basic RK schemes* $(\mathbf{b}^{\{2\}}, \mathbf{A}^{\{2,1\}}), \ldots, (\mathbf{b}^{\{N\}}, \mathbf{A}^{\{N,1\}})$*, together with the choice of* $\mathbf{b}^{\{1\}}$ *defines the partitioned symplectic GARK scheme* (3.2)*. It can be described by its Butcher tableau*

$$\begin{array}{c|ccc}
 & \hat{\mathbf{A}}^{\{2,1\}} & \ldots & \hat{\mathbf{A}}^{\{2,1\}} \\
\mathbf{A}^{\{1,2\}} & & & \\
\vdots & & & \\
\mathbf{A}^{\{1,N\}} & & & \\
\hline
\mathbf{b}^{\{1\}T} & \hat{\mathbf{b}}^{\{2\}T} & \ldots & \hat{\mathbf{b}}^{\{N\}T}
\end{array}$$

with

$$\begin{aligned}
\hat{\mathbf{A}}^{\{1,m\}} &:= \mathbb{1}\,\hat{\mathbf{b}}^{\{m\}T} - \left(\mathbf{B}^{\{1\}}\right)^{-1}\mathbf{A}^{\{m,1\}T}\hat{\mathbf{B}}^{\{m\}}, \quad m = 2, \ldots, N \\
\hat{\mathbf{b}}^{\{m\}} &:= \mathbf{b}^{\{m\}}, \quad m = 2, \ldots, N.
\end{aligned}$$

3.2. Partitioned symplectic GARK schemes for kinetic and potential splitting. The partitioned RK schemes derived in the previous subsection can be generalized to define partitioned symplectic GARK schemes for both kinetic and potential splitting. If each of the components of the right hand side of system (2.1) is further partitioned by positions and momenta components, i.e.,

$$H(p,q) = \sum_{i=1}^{2N} H^{\{i\}}(p,q) \quad \text{with } H^{\{i\}}(p,q) = T^{\{i\}}(p), \quad H^{\{N+i\}}(p,q) = U^{\{i\}}(q)$$

for $i = 1, \dots, N$, the GARK scheme (2.2) becomes

$$
\begin{aligned}
\tilde{P}_i^{\{q\}} &= p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \tilde{a}_{i,j}^{\{q,N+m\}} \tilde{k}_j^{\{N+m\}}, \\
\tilde{Q}_i^{\{q\}} &= q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \tilde{a}_{i,j}^{\{q,m\}} \tilde{\ell}_j^{\{m\}}, \\
p_1 &= p_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} \tilde{b}_i^{\{N+q\}} \tilde{k}_i^{\{N+q\}}, \\
q_1 &= q_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} \tilde{b}_i^{\{q\}} \tilde{\ell}_i^{\{q\}}, \\
\tilde{k}_i^{\{N+m\}} &= -\frac{\partial H^{\{N+m\}}}{\partial q} \left(\tilde{P}_i^{\{N+m\}}, \tilde{Q}_i^{\{N+m\}} \right) = -U^{\{m\}\prime}(\tilde{Q}_m^{\{N+m\}}), \\
\tilde{\ell}_i^{\{m\}} &= \frac{\partial H^{\{m\}}}{\partial p} \left(\tilde{P}_i^{\{m\}}, \tilde{Q}_i^{\{m\}} \right) = T^{\{m\}\prime}(\tilde{P}_i^{\{m\}}).
\end{aligned}
$$

One notes that the stage vectors $\tilde{Q}_i^{\{\ell\}}$ and $\tilde{P}_i^{\{N+\ell\}}$ are not needed for $\ell = 1, \dots, N$. Denoting

$$
\hat{\mathbf{A}}^{\{\ell,m\}} := \tilde{\mathbf{A}}^{\{\ell,N+m\}}, \quad \mathbf{A}^{\{\ell,m\}} := \tilde{\mathbf{A}}^{\{N+\ell,m\}}, \quad \hat{\mathbf{b}}^{\{\ell\}} := \tilde{\mathbf{b}}^{\{\ell\}}, \quad \mathbf{b}^{\{\ell\}} := \tilde{\mathbf{b}}^{\{N+\ell\}},
$$

the partitioned GARK scheme reads (with $P_i^{\{m\}} := \tilde{P}_i^{\{m\}}$, $Q_i^{\{m\}} := \tilde{Q}_i^{\{N+m\}}$ and $\hat{s}^{\{q\}} := s^{\{N+q\}}$)

$$
\begin{aligned}
P_i^{\{q\}} &= p_0 + h \sum_{m=1}^{N} \sum_{j=1}^{\hat{s}^{\{m\}}} \hat{a}_{i,j}^{\{q,m\}} k_j^{\{m\}}, \qquad i = 1, \dots, s^{\{q\}}, \\
Q_i^{\{q\}} &= q_0 + h \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} \ell_j^{\{m\}}, \qquad i = 1, \dots, \hat{s}^{\{q\}}, \\
p_1 &= p_0 + h \sum_{q=1}^{N} \sum_{i=1}^{\hat{s}^{\{q\}}} \hat{b}_i^{\{q\}} k_i^{\{q\}}, \\
q_1 &= q_0 + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \ell_i^{\{q\}}, \\
k_i^{\{m\}} &= -\frac{\partial H^{\{m\}}}{\partial q} \left(P_i^{\{m\}}, Q_i^{\{m\}} \right) = -U^{\{m\}\prime}(Q_i^{\{m\}}), \\
\ell_i^{\{m\}} &= \frac{\partial H^{\{m\}}}{\partial p} \left(P_i^{\{m\}}, Q_i^{\{m\}} \right) = T^{\{m\}\prime}(P_i^{\{m\}}).
\end{aligned}
$$

This scheme can also be analyzed in the framework presented in this section. The corresponding generalized Butcher tableau is

$$
\begin{array}{cc}
 & \hat{\mathbf{A}} \\
\mathbf{A} & \\
\hline
\mathbf{b} & \hat{\mathbf{b}}
\end{array}
\tag{3.6}
$$

with

$$\mathbf{A} := \begin{matrix} \mathbf{A}^{\{1,1\}} & \mathbf{A}^{\{1,2\}} & \dots & \mathbf{A}^{\{1,N\}} \\ \mathbf{A}^{\{2,1\}} & \mathbf{A}^{\{2,2\}} & \dots & \mathbf{A}^{\{2,N\}} \\ \vdots & \vdots & & \vdots \\ \mathbf{A}^{\{N,1\}} & \mathbf{A}^{\{N,2\}} & \dots & \mathbf{A}^{\{N,N\}} \end{matrix}, \quad \hat{\mathbf{A}} := \begin{matrix} \hat{\mathbf{A}}^{\{1,1\}} & \hat{\mathbf{A}}^{\{1,2\}} & \dots & \hat{\mathbf{A}}^{\{1,N\}} \\ \hat{\mathbf{A}}^{\{2,1\}} & \hat{\mathbf{A}}^{\{2,2\}} & \dots & \hat{\mathbf{A}}^{\{2,N\}} \\ \vdots & \vdots & & \vdots \\ \hat{\mathbf{A}}^{\{N,1\}} & \hat{\mathbf{A}}^{\{N,2\}} & \dots & \hat{\mathbf{A}}^{\{N,N\}} \end{matrix}, \text{ and}$$

$$\mathbf{b} := \mathbf{b}^{\{1\}} \quad \mathbf{b}^{\{2\}} \quad \dots \quad \mathbf{b}^{\{N\}}, \quad \hat{\mathbf{b}} := \hat{\mathbf{b}}^{\{1\}} \quad \hat{\mathbf{b}}^{\{2\}} \quad \dots \quad \hat{\mathbf{b}}^{\{N\}}.$$

As $\tilde{k}_i^{\{\ell\}} = 0$ and $\tilde{\ell}_i^{\{N+\ell\}} = 0$ for $\ell = 1, \dots, N$ holds, only the terms

$$d\tilde{k}_i^{\{\ell\}} \wedge d\tilde{l}_i^{\{m\}} \quad \text{for } m = 1, \dots, N; \ell = N+1, \dots, 2N$$

do not vanish, and only $\mathbf{P}^{\{N+m,\ell\}} = 0$ has to be demanded to get a symplectic scheme according to Theorem 2.1, which reads

$$\begin{aligned} &\mathbf{P}^{\{N+m,\ell\}} = 0 \\ &\Leftrightarrow (\tilde{\mathbf{A}}^{\{\ell,N+m\}})^T \mathbf{B}^{\{\ell\}} + \tilde{\mathbf{B}}^{\{N+m\}} \tilde{\mathbf{A}}^{\{N+m,\ell\}} - \tilde{\mathbf{b}}^{\{N+m\}} (\tilde{\mathbf{b}}^{\{\ell\}})^T = 0 \\ &\Leftrightarrow \hat{\mathbf{A}}^{\{\ell,m\}T} \, \hat{\mathbf{B}}^{\{\ell\}} + \mathbf{B}^{\{m\}} \, \mathbf{A}^{\{m,\ell\}} - \mathbf{b}^{\{m\}} \, \hat{\mathbf{b}}^{\{\ell\}T} = 0. \end{aligned} \tag{3.7}$$

This equation can be solved for $\hat{\mathbf{A}}^{\{\ell,m\}}$ to obtain:

$$\hat{\mathbf{A}}^{\{\ell,m\}} = \hat{\mathbf{B}}^{\{\ell\}-1} \, \hat{\mathbf{b}}^{\{\ell\}} \, \mathbf{b}^{\{m\}T} - \hat{\mathbf{B}}^{\{\ell\}-1} \, \mathbf{A}^{\{m,\ell\}T} \, \mathbf{B}^{\{m\}} = \mathbf{1} \, \mathbf{b}^{\{m\}T} - \hat{\mathbf{B}}^{\{\ell\}-1} \, \mathbf{A}^{\{m,\ell\}T} \, \mathbf{B}^{\{m\}}. \tag{3.8}$$

We note that if the weights $\mathbf{b}$ and $\bar{\mathbf{b}}$ are the same, $\hat{\mathbf{A}}^{\{\ell,m\}}$ is fixed:

$$\hat{\mathbf{A}}^{\{\ell,m\}} = \mathbf{1} \, \mathbf{b}^{\{m\}T} - \mathbf{B}^{\{\ell\}-1} \, \mathbf{A}^{\{m,\ell\}T} \, \mathbf{B}^{\{m\}}. \tag{3.9}$$

3.3. GARK discrete adjoints. GARK discrete adjoints were developed in [5]. As in the case of standard Runge-Kutta methods [6], if all the weights are nonzero, $b_i^{\{q\}} \neq 0$, we can reformulate the discrete GARK adjoint as another GARK method.

$$\lambda_n = \lambda_{n+1} + h_n \sum_{q=1}^{N} \sum_{j=1}^{s^{\{q\}}} \bar{b}_j^{\{q\}} \, \ell_{n,j}^{\{q\}}, \tag{3.10a}$$

$$\Lambda_{n,i}^{\{q\}} = \lambda_{n+1} + h_n \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \bar{a}_{i,j}^{\{q,m\}} \, \ell_{n,j}^{\{m\}}, \quad i = s^{\{q\}}, \dots, 1, \tag{3.10b}$$

$$\ell_{n,i}^{\{q\}} = \mathbf{J}_{n,i}^{\{q\}} \, \Lambda_{n,i}^{\{q\}}, \tag{3.10c}$$

with

$$\bar{b}_i^{\{q\}} = b_i^{\{q\}}, \qquad \bar{a}_{i,j}^{\{q,m\}} = \frac{b_j^{\{m\}} \, a_{j,i}^{\{m,q\}}}{b_i^{\{q\}}}. \tag{3.10d}$$

Reverting the time $h_n \to -h_n$ the stage equations (3.10b) read:

$$\Lambda_{n,i}^{\{q\}} = \lambda_n + h_n \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \bar{b}_j^{\{m\}} \, \ell_{n,j}^{\{m\}} - h_n \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \bar{a}_{i,j}^{\{q,m\}} \, \ell_{n,j}^{\{m\}}$$
$$= \lambda_n + h_n \sum_{m=1}^{N} \sum_{j=1}^{s^{\{m\}}} \hat{a}_{i,j}^{\{q,m\}} \, \ell_{n,j}^{\{m\}},$$
$$\hat{a}_{i,j}^{\{q,m\}} = \bar{b}_j^{\{m\}} - \bar{a}_{i,j}^{\{m,q\}} = b_j^{\{m\}} - \frac{b_j^{\{m\}} \, a_{j,i}^{\{m,q\}}}{b_i^{\{q\}}},$$

which reads in matrix notation

$$\hat{\mathbf{A}}^{\{q,m\}} = \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathbf{B}^{\{q\}-1}\,\mathbf{A}^{\{m,q\}T}\,\mathbf{B}^{\{m\}}$$

and is equivalent to the symplecticeness condition (3.9) of partitioned GARK schemes. The matrix

$$\hat{\mathbf{A}}^{\{q,m\}} := \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathbf{B}^{\{q\}-1}\,\mathbf{A}^{\{m,q\}T}\,\mathbf{B}^{\{m\}}$$

is called the symplectic conjugate of $\mathbf{A}^{\{q,m\}}$. If $\mathbf{A}^{\{q,m\}} = \hat{\mathbf{A}}^{\{q,m\}}$ holds, the matrix $\mathbf{A}^{\{q,m\}}$ is called self-adjoint.

In addition we have the following result:

LEMMA 3.1. *Symplecticity and self-adjointness of a GARK scheme* $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}})$ *are equivalent.*

Proof. a) Let us assume that the GARK scheme is symplectic, i.e., (1.8) holds. Then we get

$$\hat{\mathbf{A}}^{\{l,m\}} = \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathbf{B}^{\{\ell\}-1}\,\mathbf{A}^{\{m,\ell\}T}\,\mathbf{B}^{\{m\}}$$

by definition of the symplectic conjugate scheme, which is equal to $\mathbf{A}^{\{m,n\}}$), as $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}})$ is symplectic.

b) Let us assume that the GARK scheme is self-adjoint, i.e., $\mathbf{A}^{\{l,m\}} = \hat{\mathbf{A}}^{\{l,m\}}$. This yields

$$\mathbf{A}^{\{l,m\}} = \hat{\mathbf{A}}^{\{l,m\}} \Leftrightarrow \mathbf{A}^{\{l,m\}} = \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathbf{B}^{\{\ell\}-1}\,\mathbf{A}^{\{m,\ell\}T}\,\mathbf{B}^{\{m\}}$$

by definition of the symplectic conjugate scheme, which yields the symplecticity condition (1.8) when multiplying both sides with $\mathbf{B}^{\{l\}}$ from the left-hand side. ☐

As for all adjoint schemes, the order of a GARK scheme and its adjoint scheme coincide.

REMARK 8. *Sanz-Serna [8] considers Lagrangian problems:*

$$\int \mathcal{L}(q, \dot{q}, t) \to \min, \quad \mathcal{L}(q, \dot{q}, t) = T(q, \dot{q}, t) - U(q, t),$$

where the control co-states are equivalent to momenta:

$$p = \nabla_{\dot{q}}\, \mathcal{L}(q, \dot{q}, t).$$

Zanna [11] has shown that integrating the states $Q^{\{m\}}$ *with a GARK scheme, and the co-states* $P^{\{m\}}$ *with the discrete adjoint of the GARK method* (3.10) *results in a symplectic numerical method. This result generates the results of Sanz-Serna [8] for RK methods to GARK methods.*

3.4. Order conditions. According to (2.4), the order conditions of partitioned GARK schemes given by the Butcher tableau (3.6) are given by

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{1}^{\{\sigma\}} = 1, \quad \forall\, \sigma. \qquad \text{(order 1)} \tag{3.11a}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{1}^{\{\sigma\}} = 1, \quad \forall\, \sigma. \qquad \text{(order 1)} \tag{3.11b}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{c}^{\{\sigma,\nu\}} = \frac{1}{2}, \quad \forall\, \sigma,\nu, \qquad \text{(order 2)} \tag{3.11c}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \hat{\mathbf{c}}^{\{\sigma,\nu\}} = \frac{1}{2}, \quad \forall\, \sigma,\nu, \qquad \text{(order 2)} \tag{3.11d}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma,\nu\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right) = \frac{1}{3}, \quad \forall\, \sigma,\nu,\mu, \qquad \text{(order 3)} \tag{3.11e}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \left(\hat{\mathbf{c}}^{\{\sigma,\nu\}} \times \hat{\mathbf{c}}^{\{\sigma,\mu\}}\right) = \frac{1}{3}, \quad \forall\, \sigma,\nu,\mu, \qquad \text{(order 3)} \tag{3.11f}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \hat{\mathbf{c}}^{\{\nu,\mu\}} = \frac{1}{6}, \quad \forall\, \sigma,\nu,\mu, \qquad \text{(order 3)} \tag{3.11g}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \hat{\mathbf{A}}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu,\mu\}} = \frac{1}{6}, \quad \forall\, \sigma,\nu,\mu, \qquad \text{(order 3)} \tag{3.11h}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \left(\mathbf{c}^{\{\sigma,\nu\}} \times \mathbf{c}^{\{\sigma,\lambda\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right) = \frac{1}{4}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11i}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \left(\hat{\mathbf{c}}^{\{\sigma,\nu\}} \times \hat{\mathbf{c}}^{\{\sigma,\lambda\}} \times \hat{\mathbf{c}}^{\{\sigma,\mu\}}\right) = \frac{1}{4}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11j}$$

$$\left(\mathbf{b}^{\{\sigma\}} \times \mathbf{c}^{\{\sigma,\mu\}}\right)^{\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \hat{\mathbf{c}}^{\{\nu,\lambda\}} = \frac{1}{8}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11k}$$

$$\left(\hat{\mathbf{b}}^{\{\sigma\}} \times \hat{\mathbf{c}}^{\{\sigma,\mu\}}\right)^{\mathrm{T}} \cdot \hat{\mathbf{A}}^{\{\sigma,\nu\}} \cdot \mathbf{c}^{\{\nu,\lambda\}} = \frac{1}{8}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11l}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \left(\hat{\mathbf{c}}^{\{\nu,\lambda\}} \times \hat{\mathbf{c}}^{\{\nu,\mu\}}\right) = \frac{1}{12}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11m}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \hat{\mathbf{A}}^{\{\sigma,\nu\}} \cdot \left(\mathbf{c}^{\{\nu,\lambda\}} \times \mathbf{c}^{\{\nu,\mu\}}\right) = \frac{1}{12}, \quad \forall\, \sigma,\nu,\lambda,\mu, \qquad \text{(order 4)} \tag{3.11n}$$

$$\mathbf{b}^{\{\sigma\}\,\mathrm{T}} \cdot \mathbf{A}^{\{\sigma,\nu\}} \cdot \hat{\mathbf{A}}^{\{\nu,\lambda\}} \cdot \mathbf{c}^{\{\lambda,\mu\}} = \frac{1}{24}, \quad \forall\, \sigma,\nu,\lambda,\mu. \qquad \text{(order 4)} \tag{3.11o}$$

$$\hat{\mathbf{b}}^{\{\sigma\}\,\mathrm{T}} \cdot \hat{\mathbf{A}}^{\{\sigma,\nu\}} \cdot \mathbf{A}^{\{\nu,\lambda\}} \cdot \hat{\mathbf{c}}^{\{\lambda,\mu\}} = \frac{1}{24}, \quad \forall\, \sigma,\nu,\lambda,\mu. \qquad \text{(order 4)} \tag{3.11p}$$

Assume that the GARK scheme $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}})$ has order p, then $(\mathbf{b}^{\{m\}}, \hat{\mathbf{A}}^{\{m,n\}})$ with $\mathbf{A}^{\{m,n\}}$ given by (3.9) as its discrete adjoint has order p, too, and the partitioned GARK scheme $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}}, \hat{\mathbf{A}}^{\{m,n\}})$ is symplectic. Thus for $p = 4$, all order conditions up to order two are fulfilled, as well as the order three conditions (3.11e), (3.11f) and the order four conditions (3.11i), (3.11j). In addition, all other coupling conditions are fulfilled. Following the lines of the proof of Theorem 2.3, we get (note that $\mathbf{b}^{\{m\}} = \hat{\mathbf{b}}^{\{m\}T}$ holds)

$$\mathbf{b}^{\{m\}T}\,(\mathbf{c}^{\{m,s\}} \times \mathbf{c}^{\{m,\ell\}}) + \mathbf{b}^{\{\ell\}T}\,\hat{\mathbf{A}}^{\{\ell,m\}}\,\mathbf{c}^{\{m,s\}} = \frac{1}{2} \Rightarrow \text{(3.11h)}$$

$$\mathbf{b}^{\{m\}T}\,(\hat{\mathbf{c}}^{\{m,s\}} \times \hat{\mathbf{c}}^{\{m,\ell\}}) + \mathbf{b}^{\{\ell\}T}\,\mathbf{A}^{\{\ell,m\}}\,\hat{\mathbf{c}}^{\{m,s\}} = \frac{1}{2} \Rightarrow \text{(3.11g)}$$

$$\mathbf{b}^{\{l\}T}\,(\mathbf{c}^{\{l,s\}} \times \mathbf{c}^{\{l,t\}}) \times \mathbf{c}^{\{l,m\}}) + \mathbf{b}^{\{m\}T}\,\hat{\mathbf{A}}^{\{m,l\}}\,(\mathbf{c}^{\{l,s\}} \times \mathbf{c}^{\{l,t\}}) = \frac{1}{3} \Rightarrow \text{(3.11n)}$$

$$\mathbf{b}^{\{l\}T}\,(\hat{\mathbf{c}}^{\{l,s\}} \times \hat{\mathbf{c}}^{\{l,t\}}) \times \hat{\mathbf{c}}^{\{l,m\}}) + \mathbf{b}^{\{m\}T}\,\mathbf{A}^{\{m,l\}}\,(\hat{\mathbf{c}}^{\{l,s\}} \times \hat{\mathbf{c}}^{\{l,t\}}) = \frac{1}{3} \Rightarrow \text{(3.11m)}$$

$$\mathbf{b}^{\{m\}T}\,(\mathbf{A}^{\{m,s\}}\,\hat{\mathbf{c}}^{\{s,l\}} \times \mathbf{c}^{\{m,t\}}) + \mathbf{b}^{\{t\}T}\,\hat{\mathbf{A}}^{\{t,m\}}\,\mathbf{A}^{\{m,s\}}\,\hat{c}^{\{s,l\}} = \frac{1}{6}$$
$$\Rightarrow \text{(3.11k) and (3.11p) are equivalent}$$

$$\mathbf{b}^{\{m\}T}\,(\hat{\mathbf{A}}^{\{m,s\}}\,\mathbf{c}^{\{s,l\}} \times \hat{\mathbf{c}}^{\{m,t\}}) + \mathbf{b}^{\{t\}T}\,\mathbf{A}^{\{t,m\}}\,\hat{\mathbf{A}}^{\{m,s\}}\,\mathbf{c}^{\{s,l\}} = \frac{1}{6}$$
$$\Rightarrow \text{(3.11l) and (3.11o) are equivalent}$$

$$\mathbf{b}^{\{l\}T}\,(\mathbf{c}^{\{l,m\}} \times \mathbf{A}^{\{l,t\}}\,\hat{\mathbf{c}}^{\{t,s\}}) + \mathbf{b}^{\{t\}T}\,(\hat{\mathbf{c}}^{\{t,s\}} \times \hat{\mathbf{A}}^{\{t,l\}}\,\mathbf{c}^{\{l,m\}}) = \frac{1}{4}$$
$$\Rightarrow \text{(3.11k) and (3.11l) are equivalent}$$

Thus only one of the coupling conditions (3.11k) and (3.11l) remains. Thus we have shown the

THEOREM 3.2. *The partitioned GARK scheme defined by* $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}}, \hat{A}^{\{m,n\}})$*, with* $\mathbf{A}^{\{m,n\}}$ *given by* (3.9)*, has order four, iff the GARK scheme* $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,n\}}$ *has order four and either the coupling condition* (3.11k) *or* (3.11l) *holds.*

EXAMPLE 3. *The Verlet algorithm (the two-stage Lobatto IIIA–IIIB pair of order 2) has this form with* $N=1$ *and*

$$\begin{array}{c|c} \widehat{c} & \widehat{A} \\ \hline & \widehat{b}^T \end{array} := \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}, \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} := \begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array},$$

and the three-stage Lobatto IIIA–IIIB pair of order 4 is

$$\begin{array}{c|c} \widehat{c} & \widehat{A} \\ \hline & \widehat{b}^T \end{array} := \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/2 & 5/24 & 1/3 & -1/24 \\ 1 & 1/6 & 2/3 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}, \qquad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} := \begin{array}{c|ccc} 0 & 1/6 & -1/6 & 0 \\ 1/2 & 1/6 & 1/3 & 0 \\ 1 & 1/6 & 5/6 & 0 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}.$$

3.5. Symmetry and time-reversibility. The symmetry and time-reversible results for GARK scheme can be adapted to partationed GARK scheme as follows:

THEOREM 3.3 (Symmetric partitioned GARK schemes). *The partitioned GARK scheme*(3.5) *is symmetric if the following conditions on the method coefficients hold for all* $q, m = 1, \ldots, N$*:*

$$\begin{aligned} b_j^{\{q\}} &= b_{s+1-j}^{\{q\}}, \qquad j = 1, \ldots, \hat{s}^{\{q\}}, \\ a_{i,j}^{\{m,q\}} &= b_j^{\{q\}} - a_{s^{\{m\}}+1-i,\hat{s}^{\{q\}}+1-j}^{\{m,q\}}, \qquad i = 1, \ldots, s^{\{m\}},\ j = 1, \ldots, \hat{s}^{\{q\}}, \\ \widehat{b}_j^{\{q\}} &= \widehat{b}_{s+1-j}^{\{q\}}, \qquad j = 1, \ldots, s^{\{q\}}, \\ \widehat{a}_{i,j}^{\{m,q\}} &= \widehat{b}_j^{\{q\}} - \widehat{a}_{\hat{s}^{\{m\}}+1-i,s^{\{q\}}+1-j}^{\{m,q\}}, \qquad i = 1, \ldots, \hat{s}^{\{m\}},\ j = 1, \ldots, s^{\{q\}}. \end{aligned}$$

holds.

Proof. The result follows immediately from the proof for symmetric GARK schemes. ∎

REMARK 9. *The proof of Theorem 2.6 shows that symmetric partitioned GARK scheme are time-reversible.*

REMARK 10 (Time-reversed partitioned GARK method). *The time-reversed partioned GARK method is defined by*

$$\underline{\mathbf{b}}^{\{m\}} := \mathcal{P}\,\mathbf{b}^{\{m\}}, \quad \underline{\hat{\mathbf{b}}}^{\{m\}} := \mathcal{P}\,\hat{\mathbf{b}}^{\{m\}}, \tag{3.13a}$$

$$\underline{\mathbf{A}}^{\{\ell,m\}} := \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P}, \quad \underline{\hat{\mathbf{A}}}^{\{\ell,m\}} := \mathbf{1}\,\hat{\mathbf{b}}^{\{m\}T} - \mathcal{P}\,\hat{\mathbf{A}}^{\{\ell,m\}}\,\mathcal{P}\,. \tag{3.13b}$$

Consider the case where the base method is symplectic (3.7). *Similar to GARK schemes, one can show that one sufficient condition for symplecticness of the time-reversed partitioned GARK scheme is given by*

$$\hat{\mathbf{b}}^{\{m\}} = \mathcal{P}\,\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}, \qquad \hat{\mathbf{b}}^{\{\ell\}} = \mathcal{P}\,\mathbf{b}^{\{\ell\}} = \underline{\mathbf{b}}^{\{\ell\}}.$$

REMARK 11 (Matrix formulation of symmetry conditions). *Let $\mathcal{P} \in \mathbb{R}^{s\times s}$ be the permutation matrix that reverses the entries of a vector. In matrix notation the symmetry equations* (3.12) *read:*

$$\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}, \quad \hat{\mathbf{b}}^{\{m\}} = \underline{\hat{\mathbf{b}}}^{\{m\}} \tag{3.14a}$$

$$\mathbf{A}^{\{\ell,m\}} = \underline{\mathbf{A}}^{\{\ell,m\}}, \quad \hat{\mathbf{A}}^{\{\ell,m\}} = \underline{\hat{\mathbf{A}}}^{\{\ell,m\}} \tag{3.14b}$$

With other words, a partitioned GARK scheme is symmetric, if the underlying GARK scheme and its discrete adjoing scheme are symmetric.

LEMMA 3.4 (Symmetry of partiotioned GARK schems). *The symmetry of a GARK scheme $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,l\}})$ immplies the symmetry of its discrete adjoint scheme $(\mathbf{b}^{\{m\}}, \hat{\mathbf{A}}^{\{m,l\}})$ and thus the symmetry of the partitioned GARK scheme $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,l\}}, \hat{\mathbf{A}}^{\{m,l\}})$.*

Proof. We only have to show that $\mathbf{A}^{\{\ell,m\}} = \underline{\mathbf{A}}^{\{\ell,m\}}$ implies $\hat{\mathbf{A}}^{\{\ell,m\}} = \underline{\hat{\mathbf{A}}}^{\{\ell,m\}}$:

$$\hat{\mathbf{A}}^{\{\ell,m\}} = \underline{\hat{\mathbf{A}}}^{\{\ell,m\}} \Leftrightarrow \hat{\mathbf{A}}^{\{\ell,m\}} = \mathbf{1}\mathbf{b}^{\{m\}\top} - \mathcal{P}\hat{\mathbf{A}}^{\{\ell,m\}}\mathcal{P},$$

which is equivalent to

$$\mathbf{1}\mathbf{b}^{\{m\}\top} - (\mathbf{B}^{\{l\}})^{-1}\mathbf{A}^{\{m,l\}\top}\mathbf{B}^{\{m\}} = \mathbf{1}\mathbf{b}^{\{m\}\top} - \mathcal{P}\left(\mathbf{1}\mathbf{b}^{\{m\}\top} - (\mathbf{B}^{\{l\}})^{-1}\mathbf{A}^{\{m,l\}\top}\mathbf{B}^{\{m\}}\right)\mathcal{P}$$

as the partitioned GARK scheme is symplectic. Multiplying with $\mathbf{B}^{\{l\}}$ and $(\mathbf{B}^{\{m\}})^{-1}$ from left and right, resp, yields

$$\mathbf{A}^{\{m,l\}\top} = \mathbf{B}^{\{l\}}\mathcal{P}\left(\mathbf{1}\mathbf{b}^{\{m\}\top} - (\mathbf{B}^{\{l\}})^{-1}\mathbf{A}^{\{m,l\}\top}\mathbf{B}^{\{m\}}\right)\mathcal{P}(\mathbf{B}^{\{m\}})^{-1}$$

With $\mathbf{B}^{\{l\}}\mathcal{P} = \mathcal{P}\mathbf{B}^{\{l\}}$ and $\mathcal{P}(\mathbf{B}^{\{m\}})^{-1} = (\mathbf{B}^{\{m\}})^{-1}\mathcal{P}$ we get

$$\mathbf{A}^{\{m,l\}\top} = \mathcal{P}\mathbf{B}^{\{l\}}\left(\mathbf{1}\mathbf{b}^{\{m\}\top} - (\mathbf{B}^{\{l\}})^{-1}\mathbf{A}^{\{m,l\}\top}\mathbf{B}^{\{m\}}\right)(\mathbf{B}^{\{m\}})^{-1}\mathcal{P} \Leftrightarrow \hat{\mathbf{A}}^{\{m,\ell\}} = \underline{\hat{\mathbf{A}}}^{\{m,\ell\}}$$

∎

REMARK 12. *This lemma provides an easy way to construct partitioned GARK schemes of order four, which are both symmetric and symplectic. One only needs a symmetric GARK scheme* $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,l\}})$ *to get a symmetric and symplectic partitioned GARK scheme* $(\mathbf{b}^{\{m\}}, \mathbf{A}^{\{m,l\}}, \hat{\mathbf{A}}^{\{m,l\}})$ *of order four — note that lemma 3.2 generally yields only order three, but order four is then given by symmetry.*

For partitioned GARK schemes, the symmetry condition (3.14b) and the sympleticness condition (3.7) give

$$\begin{aligned}\mathbf{A}^{\{\ell,m\}} &= \mathbf{1}\,\mathbf{b}^{\{m\}T} - \mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} = \mathbf{1}\,\hat{\mathbf{b}}^{\{m\}T} - \mathbf{B}^{\{\ell\}-1}\,\hat{\mathbf{A}}^{\{m,\ell\}T}\,\hat{\mathbf{B}}^{\{m\}},\\ \hat{\mathbf{A}}^{\{\ell,m\}} &= \mathbf{1}\,\hat{\mathbf{b}}^{\{m\}T} - \mathcal{P}\,\hat{\mathbf{A}}^{\{\ell,m\}}\,\mathcal{P} = \mathbf{1}\,\mathbf{b}^{\{m\}T} - \hat{\mathbf{B}}^{\{\ell\}-1}\,\mathbf{A}^{\{m,\ell\}T}\,\mathbf{B}^{\{m\}}\,.\end{aligned}$$

and condition (2.16) reads

$$\begin{aligned}\hat{\mathbf{A}}^{\{m,\ell\}T}\,\hat{\mathbf{B}}^{\{m\}} &= \mathbf{B}^{\{\ell\}}\,\mathcal{P}\,\mathbf{A}^{\{\ell,m\}}\,\mathcal{P} + \mathbf{b}^{\{\ell\}}\,(\hat{\mathbf{b}}^{\{m\}T} - \mathbf{b}^{\{m\}T}),\\ \mathbf{A}^{\{m,\ell\}T}\,\mathbf{B}^{\{m\}} &= \hat{\mathbf{B}}^{\{\ell\}}\,\mathcal{P}\,\hat{\mathbf{A}}^{\{\ell,m\}}\,\mathcal{P} + \hat{\mathbf{b}}^{\{\ell\}}\,(\mathbf{b}^{\{m\}T} - \hat{\mathbf{b}}^{\{m\}T}),\\ b_j^{\{m\}}\,a_{j,i}^{\{m,\ell\}} &= b_i^{\{\ell\}}\,\hat{a}_{s+1-i,s+1-j}^{\{\ell,m\}} \quad \text{for } \mathbf{b}^{\{m\}} = \hat{\mathbf{b}}^{\{m\}}.\end{aligned}$$

With the help of time-reversed symplectic GARK methods one can derive symmetric and symplectic GARK methods:

THEOREM 3.5. *Assume that the partitioned GARK scheme* $\mathbf{A}^{\{l,m\}}, b^{\{m\}}, \hat{\mathbf{A}}^{\{l,m\}}, \hat{b}^{\{m\}}$ *is symplectic. If* $\hat{\mathbf{b}}^{\{m\}} = \mathcal{P}\,\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}$ *and* $\mathbf{b}^{\{m\}} = \hat{\mathbf{b}}^{\{m\}}$ *hold, the partitioned GARK scheme defined by applying one step with the GARK scheme, followed by one step with its time-reversed GARK scheme, i.e.,*

$$\left(\begin{pmatrix}\mathbf{A}^{\{l,m\}} & 0\\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{l,m\}}\end{pmatrix}, \begin{pmatrix}\mathbf{b}^{\{m\}}\\ \underline{\mathbf{b}}^{\{m\}}\end{pmatrix}, \begin{pmatrix}\hat{\mathbf{A}}^{\{l,m\}} & 0\\ \mathbf{1}\hat{\mathbf{b}}^{\{m\}T} & \underline{\hat{\mathbf{A}}}^{\{l,m\}}\end{pmatrix}, \begin{pmatrix}\hat{\mathbf{b}}^{\{m\}}\\ \underline{\hat{\mathbf{b}}}^{\{m\}}\end{pmatrix}\right). \tag{3.15}$$

is both symmetric and symplectic.

Proof. For symmetry we have to show

$$\begin{pmatrix}\mathbf{A}^{\{l,m\}} & 0\\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{l,m\}}\end{pmatrix} + \begin{pmatrix}0 & \mathcal{P}\\ \mathcal{P} & 0\end{pmatrix}\begin{pmatrix}\mathbf{A}^{\{l,m\}} & 0\\ \mathbf{1}\mathbf{b}^{\{m\}T} & \underline{\mathbf{A}}^{\{l,m\}}\end{pmatrix}\begin{pmatrix}0 & \mathcal{P}\\ \mathcal{P} & 0\end{pmatrix} = \begin{pmatrix}\mathbf{1}\mathbf{b}^{\{m\}T} & \mathbf{1}\mathbf{b}^{\{m\}T}\\ \mathbf{1}\underline{\mathbf{b}}^{\{m\}T} & \mathbf{1}\underline{\mathbf{b}}^{\{m\}T}\end{pmatrix},$$

which is equivalent to $\mathcal{P}\mathbf{b}^{\{m\}} = \mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}$. The same applies to the conjugate scheme. Symplecticeness requires

$$\begin{aligned}\begin{pmatrix}\hat{\mathbf{A}}^{\{l,m\}} & 0\\ \mathbf{1}\hat{\mathbf{b}}^{\{m\}} & \underline{\hat{\mathbf{A}}}^{\{l,m\}}\end{pmatrix} = &\begin{pmatrix}\mathbf{1}\mathbf{b}^{\{m\}} & \mathbf{1}\mathbf{b}^{\{m\}}\\ \mathbf{1}\underline{\mathbf{b}}^{\{m\}} & \mathbf{1}\underline{\mathbf{b}}^{\{m\}}\end{pmatrix} -\\ &\begin{pmatrix}\mathbf{B}^{\{l\}-1} & 0\\ 0 & \hat{\mathbf{B}}^{\{l\}-1}\end{pmatrix}\begin{pmatrix}\mathbf{A}^{\{m,l\}T} & \mathbf{b}^{\{l\}}\mathbf{1}^T\\ 0 & \underline{\mathbf{A}}^{\{m,l\}T}\end{pmatrix}\begin{pmatrix}\mathbf{B}^{\{m\}} & 0\\ 0 & \hat{\mathbf{B}}^{\{m\}}\end{pmatrix},\end{aligned}$$

which holds for a symplectic partitioned scheme $\mathbf{A}^{\{l,m\}}, \mathbf{b}^{\{m\}}, \hat{\mathbf{A}}^{\{l,m\}}, \mathbf{b}^{\{m\}}$, if $\mathbf{b}^{\{m\}} = \underline{\mathbf{b}}^{\{m\}}$. □

REMARK 13. *One drawback of this construction is the low degree of freedom* $\lceil s^{\{m\}}/2 \rceil$ *in the weights* $\mathbf{b}^{\{m\}}$.

If we aim at explicit schemes with an even number of stages $s^{\{l\}}$, a necessary property is that the matrices $\mathbf{A}^{\{l,l\}}$ are at least (after some rearrangement of stages) lower triangular matrices. Symmetry than requires the general form

$$\mathbf{A}^{\{l,l\}} = \begin{pmatrix}\left(\mathbf{1}_l\mathbf{1}_l^T - X_{l,l}\right)\tilde{\mathbf{B}}^{\{l\}} & 0\\ \mathbf{1}_l\tilde{\mathbf{b}}^{\{l\}T} & P_l\left(X_{l,l}\tilde{\mathbf{B}}^{\{l\}}\right)P_l\end{pmatrix}$$

with weights $\mathbf{b}^{\{l\}T} = (\tilde{\mathbf{b}}^{\{l\}T}, (\mathcal{P}\tilde{\mathbf{b}}^{\{l\}})^T)^T$, $\mathcal{P}_l$ being the permutation matrix of dimension $s^{\{l\}}/2$, $\tilde{B}^{\{l\}} := \mathrm{diag}(\tilde{b}^{\{l\}})$ and arbitrary matrices $X_{l,l} \in \mathbb{R}^{s^{\{l\}}/2 \times s^{\{l\}}/2}$. The conjugate scheme is given by

$$\hat{\mathbf{A}}^{\{l,l\}} = \begin{pmatrix} X_{l,l}^T \tilde{\mathbf{B}}^{\{l\}} & 0 \\ \mathbf{1}_l \tilde{\mathbf{b}}^{\{l\}T} & P_l(\mathbf{1}_l\mathbf{1}_l^T - X_{l,l}^T)\tilde{\mathbf{B}}^{\{l\}} P_l \end{pmatrix}, \quad \hat{\mathbf{b}}^{\{l\}} = \mathbf{b}^{\{l\}}.$$

To get an overall symmetric and symplectic scheme, the coupling matrices might be set by

$$\mathbf{A}^{\{l,m\}} = \begin{pmatrix} \left(\mathbf{1}_l\mathbf{1}_m^T - X_{l,m}\right)\tilde{\mathbf{B}}^{\{m\}} & 0 \\ \mathbf{1}_l \tilde{\mathbf{b}}^{\{m\}T} & P_l\left(X_{l,m}\tilde{\mathbf{B}}^{\{m\}}\right)P_m \end{pmatrix},$$

$$\hat{\mathbf{A}}^{\{l,m\}} = \begin{pmatrix} X_{m,l}^T \tilde{\mathbf{B}}^{\{m\}} & 0 \\ \mathbf{1}_l \tilde{\mathbf{b}}^{\{m\}T} & P_l(\mathbf{1}_l\mathbf{1}_m^T - X_{m,l}^T)\tilde{\mathbf{B}}^{\{m\}} P_m \end{pmatrix}.$$

REMARK 14. *This construction is equivalent to the construction of Theorem 2.5 with choosing symmetric matrices* $\mathbf{A}^{\{l,m\}} := \left(\mathbf{1}_l\mathbf{1}_m^T - X_{l,m}\right)\tilde{\mathbf{B}}^{\{m\}}$ *and* $\hat{\mathbf{A}}^{\{l,m\}} := X_{m,l}^T\tilde{\mathbf{B}}^{\{m\}}$ *based on time-reversed schemes, if* $\mathcal{P}\tilde{\mathbf{b}}^{\{m\}} = \tilde{\mathbf{b}}^{\{m\}}$ *holds. However, this construction allows for arbitrary weights* $\mathbf{b}^{\{m\}}$ *to keep the degree of freedom* $s^{\{m\}}$ *in these weigths.*

4. Symplectic and time-reversible GARK schemes for Hamiltonians with multirate potential. Consider a Hamiltonian $H(p,q) = T(p) + V(q)$, where the potential can be split into two parts $V(q) = V_1(q) + V_2(q)$. Assuming that V_1 is characterized by a fast dynamics and cheap evaluation costs, and V_2 by a slow dynamics and expensive evaluation costs, resp. Then the Hamiltion can be partitioned into two parts $H_1(p,q) = T(p) + V_1(q)$ and $H_2(p,q) = V_2(q)$ with fast/slow dynamics and cheap/expensive evaluation costs, resp. The partitioned GARK scheme (3.5) for this setting reads

$$\begin{aligned}
P_i^{\{1\}} &= p_0 + h\left(\sum_{j=1}^{\hat{s}^{\{1\}}} \hat{a}_{i,j}^{\{1,1\}} k_j^{\{1\}} + \sum_{j=1}^{\hat{s}^{\{2\}}} \hat{a}_{i,j}^{\{1,2\}} k_j^{\{2\}}\right), \qquad i = 1,\dots,s^{\{1\}},\\
Q_i^{\{1\}} &= q_0 + h\sum_{j=1}^{s^{\{1\}}} a_{i,j}^{\{1,1\}} \ell_j^{\{1\}}, \qquad i = 1,\dots,\hat{s}^{\{1\}},\\
Q_i^{\{2\}} &= q_0 + h\sum_{j=1}^{s^{\{1\}}} a_{i,j}^{\{2,1\}} \ell_j^{\{1\}}, \qquad i = 1,\dots,\hat{s}^{\{2\}},\\
p_1 &= p_0 + h\left(\sum_{i=1}^{\hat{s}^{\{1\}}} \hat{b}_i^{\{1\}} k_i^{\{1\}} + \sum_{i=1}^{\hat{s}^{\{2\}}} \hat{b}_i^{\{2\}} k_i^{\{2\}}\right),\\
q_1 &= q_0 + h\sum_{i=1}^{s^{\{1\}}} b_i^{\{1\}} \ell_i^{\{1\}},\\
k_i^{\{m\}} &= -\frac{\partial H^{\{m\}}}{\partial q}\left(P_i^{\{m\}}, Q_i^{\{m\}}\right) = -U^{\{m\}\prime}(Q_i^{\{m\}}), \qquad m = 1,2,\\
\ell_i^{\{1\}} &= \frac{\partial H^{\{1\}}}{\partial p}\left(P_i^{\{1\}}, Q_i^{\{1\}}\right) = T^{\{1\}\prime}(P_i^{\{1\}}).
\end{aligned}$$

with an even number of $s^{\{1\}} = \hat{s}^{\{1\}}$ and $\hat{s}^{\{2\}}$ (with $\hat{s}^{\{2\}} \le s^{\{1\}}$) stages one gets an explicit symmetric scheme, if the stage vectors are computed in the following order:

$$\begin{aligned}
&P_1^{\{1\}}, Q_1^{\{1\}}, Q_1^{\{2\}}, \dots, P_{\hat{s}^{\{2\}}/2}^{\{1\}}, Q_{\hat{s}^{\{2\}}/2}^{\{1\}}, Q_{\hat{s}^{\{2\}}/2}^{\{2\}},\\
&P_{\hat{s}^{\{2\}}/2+1}^{\{1\}}, Q_{\hat{s}^{\{2\}}/2+1}^{\{1\}}, \dots, P_{s^{\{1\}}/2}^{\{1\}}, Q_{s^{\{1\}}/2}^{\{1\}},\\
&Q_{s^{\{1\}}/2+1}^{\{1\}}, P_{s^{\{1\}}/2+1}^{\{1\}}, \dots, Q_{s^{\{1\}}-\hat{s}^{\{2\}}/2}^{\{1\}}, P_{s^{\{1\}}-\hat{s}^{\{2\}}/2}^{\{1\}},\\
&Q_{s^{\{1\}}-\hat{s}^{\{2\}}/2+1}^{\{1\}}, Q_{\hat{s}^{\{2\}}/2+1}^{\{2\}}, P_{s^{\{1\}}-\hat{s}^{\{2\}}/2+1}^{\{1\}}, \dots, Q_{s^{\{1\}}}^{\{1\}}, Q_{\hat{s}^{\{2\}}}^{\{2\}}, P_{s^{\{1\}}}^{\{1\}}
\end{aligned}$$

For $s^{\{1\}} = 6$ and $\hat{s}^{\{2\}} = 2$ stages this coincides with the choice

$$X_{1,1} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_{1,2} = X_{2,1} = \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}.$$

in remark 13. One gets (with the same weights for p and q)

$$\begin{aligned}
\mathbf{b}^{\{1\}\top} = \hat{\mathbf{b}}^{\{1\}\top} &= \begin{pmatrix} b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & b_2^{\{1\}} & b_1^{\{1\}} \end{pmatrix}^\top,\\
\mathbf{b}^{\{2\}\top} := \hat{\mathbf{b}}^{\{2\}\top} &= \begin{pmatrix} b_1^{\{2\}} & b_1^{\{2\}} \end{pmatrix}^\top,
\end{aligned}$$

$$\hat{\mathbf{A}}^{\{1,1\}} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & 0 & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & b_2^{\{1\}} & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & b_2^{\{1\}} & b_1^{\{1\}} \end{pmatrix}, \hat{\mathbf{A}}^{\{1,2\}} = \begin{pmatrix} 0 & 0 \\ b_1^{\{2\}} & 0 \\ b_1^{\{2\}} & 0 \\ b_1^{\{2\}} & 0 \\ b_1^{\{2\}} & 0 \\ b_1^{\{2\}} & b_1^{\{2\}} \end{pmatrix},$$

and symplecticness yields

$$\begin{aligned}
\mathbf{A}^{\{1,1\}} &= \begin{pmatrix} b_1^{\{1\}} & 0 & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & b_2^{\{1\}} & 0 \end{pmatrix},\\
\mathbf{A}^{\{2,1\}} &= \begin{pmatrix} b_1^{\{1\}} & 0 & 0 & 0 & 0 & 0 \\ b_1^{\{1\}} & b_2^{\{1\}} & b_3^{\{1\}} & b_3^{\{1\}} & b_2^{\{1\}} & 0 \end{pmatrix}.
\end{aligned}$$

One idea to exploit the split structure of H_1 and H_2 and to approximate the contribution of H_1 with higher order than H_2.

To get order 4 and 2, resp., the following order conditions must be fulfilled: for order one

$$\mathbf{b}^{\{1\}\top}\mathbb{1} = 1, \quad \mathbf{b}^{\{2\}\top}\mathbb{1} = 1$$

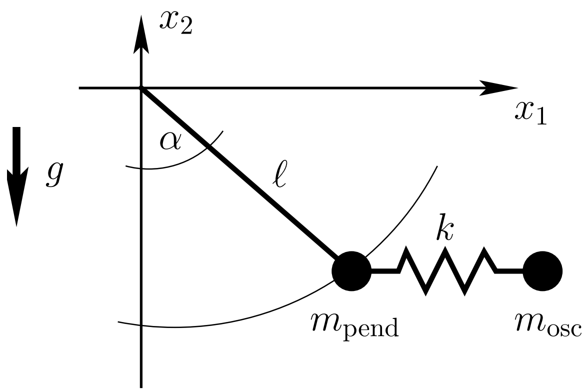

Fig. 4.1: Mathematical pendulum coupled to an oscillator (taken after [2]).

and for order three

$$\mathbf{b}^{\{1\}\top}(\hat{\mathbf{A}}^{\{1,1\}}\mathbb{1}, \hat{\mathbf{A}}^{\{1,1\}}\mathbb{1}) = \frac{1}{3},$$
$$\mathbf{b}^{\{1\}\top}\hat{\mathbf{A}}^{\{1,1\}}\hat{\mathbf{A}}^{\{1,1\}}\mathbb{1} = \frac{1}{6},$$

Note that the order conditions for order two for both H_1 and H_2 are automatically fulfilled by the order one condition,as well as for order four for H_1 by the order three condition, as the scheme is symmetric.

Remark 15. *Order* 4 *for the fast part* H_1 *cannot be obtained with less stages, as less than three degrees of freedom cannot fulfill three order conditions: for* 2 *and* 4 *stages one gets* 1 *and* 2 *degrees freedom; for* $s = 3$ *and* 5 *stages one only gets* 1 *and* 2 *degrees of freedom, resp., as one degree of freedom is lost due to the condition*

$$b^{\{l\}}_{\frac{s+1}{2}} = 2a^{\{l,l\}}_{\frac{s+1}{2},\frac{s+1}{2}} = 0$$

for explicit schemes.

The unique solution of these four order conditions for the four free parameters $b_1^{\{1\}}, b_2^{\{1\}}, b_3^{\{1\}}$ and $b_1^{\{2\}}$ is

$$b_1^{\{1\}} = 1.087752930244776,$$
$$b_2^{\{1\}} = -1.131212304665920,$$
$$b_3^{\{1\}} = 0.543459374420984,$$
$$b_1^{\{2\}} = 0.5.$$

As an example of such a system with multiscale behaviour we consider a mathematical pendulum of constant length ℓ that is coupled to a damped oscillator with a horizontal degree of freedom, as illustrated in Figure 4.1. The system consists of two rigid bodies: the first mass m_{pend} is connected to a second mass m_{osc} by a soft spring with stiffness k. Neglecting the friction of the spring, the system is Hamiltonian.

The minimal set of coordinates $q^\top = (q_1, q_2) := (\alpha, x_1)$ and generalized momenta $p^\top = (p_1, p_2)$ uniquely describe the position and momenta of both bodies. The Hamiltonian of the system is given by

$$H(q,p) = H_1(q,p) + H_2(q,p)$$

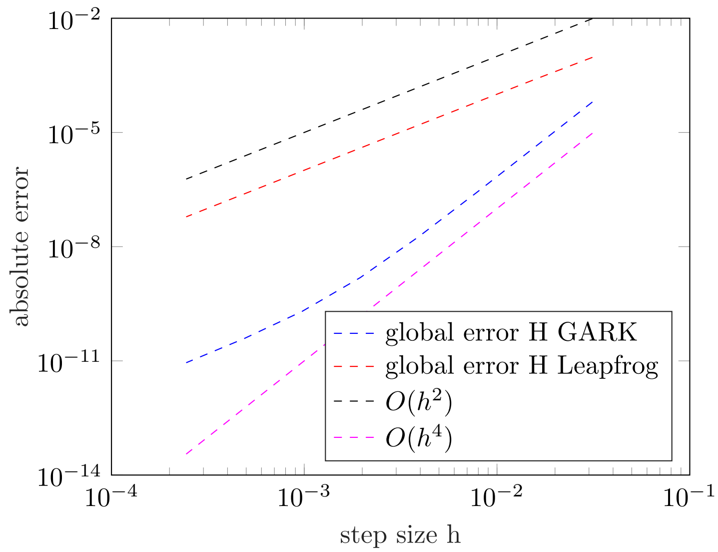

Fig. 4.2: Numerical results for parameters $m_{pend} = m_{osc} = \ell = 1$ and $k = 10^{-4}$: abolute error in the Hamiltonian H for leapfrog and symplectic scheme vs. step size.

with the fast Hamiltonian

$$\begin{aligned} H_1(q,p) &= T(p) + V_1(q), \\ T(p) &= \frac{1}{2m_{osc}} p_2^2 + \frac{1}{2m_{pend}} \left(\frac{p_1}{\ell}\right)^2, \\ V_1(q) &= -m_{pend}\, g\, \ell\, \cos(q_1), \end{aligned}$$

and the slow Hamiltonian

$$H_2(q,p) = V_2(q) = \frac{1}{2} k \left(q_2 - \ell \sin(q_1)\right)^2 .$$

The equations of motion are then given by the second-order ODE system

$$\begin{pmatrix} m_{\text{pend}}\, \ell & 0 \\ 0 & m_{\text{osc}} \end{pmatrix} \ddot{q} = \begin{pmatrix} -m_{\text{pend}}\, g\, \sin(\alpha) + \cos(\alpha)\, F \\ -F \end{pmatrix} =: f(q),$$

with the abbreviation

$$F = k\left(x_1 - \ell\, \sin(\alpha)\right)$$

for the spring force.

Figures 4.2 and 4.3 show the numerical results obtained for this benchmark for both the symplectic GARK scheme and — for comparision — the leapfrog scheme.

The results can be explained as follows: the symplectic GARK scheme yields an error expansion with an order two term due to V_2 and an order four term due to V_1, as the Hamiltonian H_1 and H_2 are solved with fourth and second order accuracy, resp.

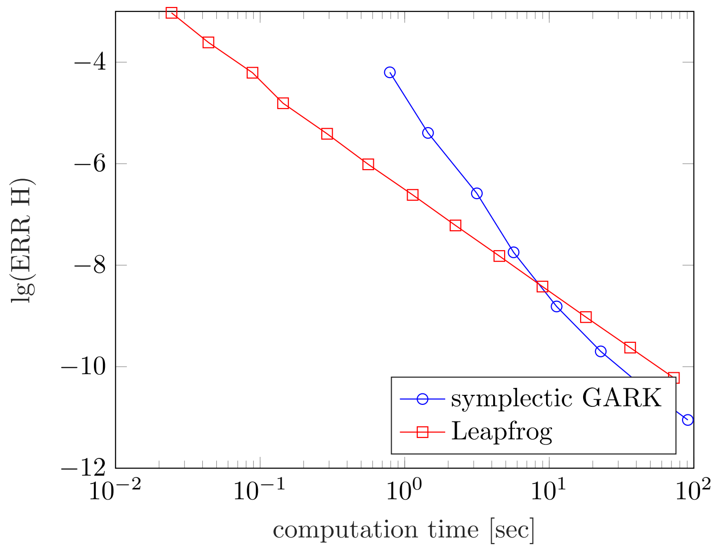

Fig. 4.3: Numerical results for parameters $m_{pend} = m_{osc} = \ell = 1$ and $k = 10^{-4}$: asbolute error in the Hamiltonian H for leapfrog and symplectic scheme vs. compuation time.

For large step sizes the fourth error term dominates, for smaller step sizes the second order term. This explains the slopes 4 and 2 visible in Fig. 4.2 for the symplectic GARK scheme for large and small step sizes, resp. As one can see in Fig. 4.3, the symplectic GARK scheme becomes advantageous for higher accuracy demands in terms of computation time. Compared to the fourth-order scheme of Yoshida [10], which has to use three function evaluations per step, the symplectic GARK scheme only needs two function evaluations for the slow, but expensive part V_2 per step.

5. Conclusions. In this paper we have derived symplectic GARK schemes in the GARK framework, which allow for arbitrary splitting of the Hamiltonian into different Hamiltonian systems. The derived symplecticity conditions reduce drastically the number of GARK order conditions. We show that symmetric GARK schemes are time-reversible and construct symmetric and time-reversible GARK schemes based on a symplectic GARK scheme and its time-reversed scheme. A special attention is given to partitioned symplectic GARK schemes, which can be tailored to a specific splitting w.r.t. potentials or potentials and kinetic parts, resp. We show that symplecticity and self-adjointness are equivalent, and show how the coupling matrices $\mathbf{A}^{l,m}$ and $\hat{\mathbf{A}}^{l,m}$ can be chosen to guarantee explicit schemes. Using different orders for different parts of the splitting defines one way to exploit the multirate behaviour given by different potentials V_1 and V_2 of a Hamiltonian, where V_1 is characterized by a fast dynamics and cheap evaluation costs, and V_2 by a slow dynamics and expensive evaluation costs, resp. Numerical tests for a coupled oscillator verify the theoretical results.

Next steps will be to derive tailored symplectic GARK schemes for specific couplings arising in applications on the one hand, and to generalize symplectic GARK schemes to multirate symplectic GARK schemes, which use different step sizes for different partitions to exploit the multirate potential. Another task will be to generalize this Abelian setting to a Non-Abelian setting used in lattice QCD, for example, where the equations of motion are defined on Lie groups and their associated Lie algebras.

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Apendix.

Proof of 2.1 based on differential forms. We have to show that

$$\sum_{J=1}^{d} dp_1^J \wedge dq_1^J = \sum_{J=1}^{d} dp_0^J \wedge dq_0^J,$$

where the superscript J denotes the J-th component of the respective quantity. Following the argumentation in [3], we differentiate the GARK scheme with respect to the initial values to obtain

$$\begin{aligned}
&dp_1^J \wedge dq_1^J - dp_0^J \wedge dq_0^J = \\
&= h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} dp_0^J \wedge d\ell_i^{\{q\},J} + h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} dk_i^{\{q\},J} \wedge dq_0^J + \\
&\quad h^2 \sum_{q,m=1}^{N} \sum_{i=1}^{s^{\{q\}}} \sum_{j=1}^{s^{\{m\}}} b_i^{\{q\}} b_j^{\{m\}} dk_i^{\{q\},J} \wedge d\ell_j^{\{m\},J} \\
&= h \sum_{q=1}^{N} \sum_{i=1}^{s^{\{q\}}} b_i^{\{q\}} \left(dP_i^{\{q\},J} \wedge d\ell_i^{\{q\},J} + dk_i^{\{q\},J} \wedge dQ_i^{\{q\},J} \right) \\
&\quad - h^2 \sum_{q,m=1}^{N} \sum_{i=1}^{s^{\{q\}}} \sum_{j=1}^{s^{\{m\}}} \left(b_i^{\{q\}} a_{i,j}^{\{q,m\}} + b_j^{\{m\}} a_{j,i}^{\{m,q\}} - b_i^{\{q\}} b_j^{\{m\}} \right) dk_i^{\{q\},J} \wedge d\ell_j^{\{m\},J}.
\end{aligned}$$

The last term is zero due to (1.8). Adding up the components $J = 1 \dots d$ of the summand $dP_i^{\{q\},J} \wedge d\ell_i^{\{q\},J} + dk_i^{\{q\},J} \wedge dQ_i^{\{q\},J}$, and expressing $d\ell_i^{\{q\},J}$ and $dk_i^{\{q\},J}$ by $dQ_i^{\{q\},J}$ and $dP_i^{\{q\},J}$ via (2.2f) and (2.2e), respectively, leads to

$$\sum_{J=1}^{N} \left(dP_i^{\{q\},J} \wedge d\ell_i^{\{q\},J} + dk_i^{\{q\},J} \wedge dQ_i^{\{q\},J} \right) =$$
$$\sum_{J,L=1}^{N} \frac{\partial^2 H^{\{q\}}}{\partial p^J \partial p^L} \, dP_i^{\{q\},J} \wedge dP_i^{\{q\},L} \frac{\partial^2 H^{\{q\}}}{\partial p^J \partial q^L} \, dP_i^{\{q\},J} \wedge dQ_i^{\{q\},L} +$$
$$\frac{\partial^2 H^{\{q\}}}{\partial q^J \partial p^L} \, dQ_i^{\{q\},J} \wedge dP_i^{\{q\},L} + \frac{\partial^2 H^{\{q\}}}{\partial q^J \partial q^L} \, dQ_i^{\{q\},J} \wedge dQ_i^{\{q\},L}.$$

We have omitted the arguments $(P_i^{\{q\}}, Q_i^{\{q\}})$ for simplicity of notation. The second and third terms cancel due to the symmetry of the partial derivatives and the antisymmetry of the $\wedge$-operator. The first term is

$$\sum_{J,L=1}^{d} \frac{\partial^2 H^{\{q\}}}{\partial p^J \partial p^L} dP_i^{\{q\},J} \wedge dP_i^{\{q\},L} = \sum_{J<L} \left(\frac{\partial^2 H^{\{q\}}}{\partial p^J \partial p^L} - \frac{\partial^2 H^{\{q\}}}{\partial p^L \partial p^J} \right) dP_i^{\{q\},J} \wedge dP_i^{\{q\},L}$$

due to the antisymmetry of the $\wedge$-operator, therefore is zero due to the symmetry of the derivatives. The same reasoning shows that the last term is also equal to zero. We conclude that

$$\sum_{J=1}^{d} dp_1^J \wedge dq_1^J = \sum_{J=1}^{d} dp_0^J \wedge dq_0^J \, .$$