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Approximate compositions of a near identity map by multi-revolution Runge-Kutta methods ⋆

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Summary. The so-called multi-revolution methods were introduced in celestial mechanics as an efficient tool for the long-term numerical integration of nearly periodic orbits of artificial satellites around the Earth. A multi-revolution method is an algorithm that approximates the map φ_T^N of N near-periods T in terms of the one near-period map φ_T evaluated at few $s \ll N$ selected points. More generally, multi-revolution methods aim at approximating the composition φ^N of a near identity map φ. In this paper we give a general presentation and analysis of multi-revolution Runge-Kutta (MRRK) methods similar to the one developed by Butcher for standard Runge-Kutta methods applied to ordinary differential equations. Order conditions, simplifying assumptions, and order estimates of MRRK methods are given. MRRK methods preserving constant Poisson/symplectic structures and reversibility properties are characterized. The construction of high order MRRK methods is described based on some families of orthogonal polynomials.

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1 Introduction

The so-called multi-revolution methods were introduced in celestial mechanics as an efficient tool for the long-term numerical integration of nearly periodic orbits of artificial satellites around the Earth [12, 20]. For those problems, the main force acting on the satellite is due to the leading term of the Earth's gravitational field. The position vector $r(t) \in \mathbb{R}^3$ of the satellite at time t with respect to the Earth's center is governed by a second order system of differential equations of the form $r'' = -\rho r/\|r\|^3 + P(r, r')$ where ρ is a constant depending on the units chosen and the vector P is a perturbation term small with respect to the leading force acting on the satellite. For $P \equiv 0$ this system reduces to the two-body problem and for usual initial conditions the satellite describes an elliptic orbit with a period $T = T(r(t_0), r'(t_0))$. Hence, in the perturbed problem it is expected that after one near-period T the change of the state vector $y(t) = (r(t), r'(t)) \in \mathbb{R}^6$ will be small and the one near-period map (also called return map or Poincaré map) $\varphi_T : y(t_0) \mapsto y(t_0 + T)$ will be a near identity map. In this context, multi-revolution methods attempt to track repeatedly the solution after a large number N of near-periods by using the one near-period map φ_T at a few suitable points.

In [20] Taratynova proposed several explicit multi-revolution multistep and Runge-Kutta algorithms to approximate the solution after N near-periods T using the one near-period map φ_T at few $s \ll N$ selected points. For these methods it is assumed that the one near-period map is a near identity map in some neighbourhood of an initial value and that the near-period T is fixed in advance. Clearly, these multi-revolution methods provide an efficient algorithm for $s \ll N$ if the errors in the approximation are comparable with those obtained with standard integration methods over N near-periods T.

Multi-revolution methods have been proposed for the long-term integration of more general nearly periodic problems. For example, consider an initial value problem for a sufficiently smooth system of differential equations

$$y' = g_1(y) + g_2(y), \quad y(t_0) = y_0, \tag{1}$$

so that $\|g_2\|$ is small with respect to $\|g_1\|$ and such that for all initial values u in a certain neighbourhood of y_0 the system $y' = g_1(y)$ possess periodic solutions with period $T = T(u)$. Denoting the solution of (1) by $y(t, t_0, y_0)$, by continuous dependence on the initial conditions the one near-period map $\varphi_{T(y_0)} : u \mapsto y(t_0 + T(y_0), t_0, u)$ is thus a near identity map in a neighbourhood of y_0.

Long-term integration of some multi-scale problems leads also to near identity maps. Suppose, for simplicity, a linear system $y' = Ay$ with constant coefficients such that matrix A has a pair of simple eigenvalues $\lambda = \pm i\omega$

with $|\omega| > 0$ very large with respect to the size of the remaining eigenvalues. The solution $y(t)$ of this linear system with $y(t_0) = y_0$ is given by $y(t) = \exp((t - t_0)A)y_0$. Taking $T = 2\pi/\omega \ll 1$, for all t_0 the map $\varphi_T : y_0 \mapsto y(t_0 + T) = y_0 + (\exp(TA) - I)y_0$ is thus a near identity map.

In this paper we are interested in the long-term integration of initial value problems for which it is possible to obtain a discrete near identity map from the continuous flow map. As remarked above such problems arise, e.g., in celestial mechanics [5,6,12,20]. Several authors, e.g., Taratynova [20], Petzold [16], Melendo and Palacios [14], have proposed multi-revolution (also called envelope-following in [16]) multistep methods and applied them not only to problems of celestial mechanics, but also to highly oscillatory problems which arise in other applications, such as in circuit simulation [11, 21,22]. In [14,16], some theoretical justifications of multi-revolution multistep methods have been given and other details related with their practical application such as estimating the near-period, have been studied. A recent survey paper [17] gives an account of some developments of these methods and other methods for systems of highly oscillatory differential equations. On the other hand, several explicit multi-revolution Runge-Kutta (EMRRK) methods were proposed by Taratynova [20]. Recently an extended study of EMRRK methods has been given by Calvo, Montijano, and Rández in [3], presenting some numerical examples which show that these methods can be more efficient than conventional methods in the treatment of these problems.

The aim of this paper is to give a general presentation and analysis of multi-revolution Runge-Kutta (MRRK) methods, more particularly of implicit MRRK methods, similar to the one developed by Butcher for standard RK methods [1,2,8]. The paper is organized as follows. In Sect. 2 we introduce the basic assumptions of the problems under consideration, MRRK methods are defined and their order conditions are given. In Sect. 3 simplifying assumptions are presented and order estimates of MRRK methods are obtained. In Sect. 4 we characterize MRRK methods preserving important geometric properties, such as constant Poisson/symplectic structures and reversibility properties. In Sect. 5 the construction of high order implicit MRRK methods is described based on some orthogonal polynomials. In Sect. 6 we discuss the extension of MRRK methods to non-autonomous maps. Numerical experiments with the harmonic oscillator and a nonlinear perturbation are presented in Sect. 7. Finally some conclusions are given in Sect. 8.

2 Compositions of a near identity map and MRRK methods

Let $\varphi : \mathbb{R}^m \to \mathbb{R}^m$ be a near identity map in a neighbourhood U of a given initial value $y_0 \in \mathbb{R}^m$. For n a positive integer value the map φ^n :

$\mathbb{R}^m \to \mathbb{R}^m$ is defined recursively by composing n times the map φ, i.e., $\varphi^n(y) := \varphi(\varphi^{n-1}(y))$. We assume that there exists a positive integer value $N_{\max}$ such that $\varphi^n(y_0)$ is well-defined for $n = 0, 1, \ldots, N_{\max}$. Notice that there is no restriction on $N_{\max}$ if y_0 is sufficiently close to a stable fixed point of the map φ. The aim of multi-revolution methods is to approximate $\varphi^N(y_0)$ (with $N \leq N_{\max}$), i.e., N compositions of the near identity map φ at y_0.

For the theory we assume that φ can be written in the form

$$\varphi(y) = y + \varepsilon f(y), \tag{2}$$

where ε ($0 \leq \varepsilon \ll 1$) is a small parameter and f is a sufficiently smooth function in U, more precisely we assume that in U, f and its derivatives up to a certain order $Q + 1$ are of moderate size. The T-flow map φ_T of a system of differential equations with near-period T is generally obtained approximately by means of an "inner" numerical integration method. Denoting the corresponding numerical flow map by $\widetilde{\varphi}_T$, an "outer" multirevolution method therefore approximates $\widetilde{\varphi}_T^N$. The numerical flow map $\widetilde{\varphi}_T$ must satisfy the assumptions of (2) to apply a multirevolution method on top of it. Hence, the numerical approximation $\widetilde{\varphi}_T$ must be obtained in a sufficiently smooth way. To approximate φ_T^N by using a multirevolution method based on $\widetilde{\varphi}_T$, it is also necessary for the difference $\widetilde{\varphi}_T(y) - \varphi_T(y)$ to be small compared to $\varphi_T(y) - y$.

From (2) the expression $\varphi^N(y_0)$ can be interpreted as the successive application of N steps with constant "stepsize" ε of the explicit Euler method to the auxiliary autonomous initial value problem

$$\frac{dy}{dx} = f(y), \quad y(0) = y_0. \tag{3}$$

We emphasize the fact that one is not interested in the exact solution of this initial value problem. Nonetheless, notice that for $\varepsilon = x/N$, $\varepsilon N = x$ is fixed and we have $\lim_{N\to\infty} \varphi^N(y_0) = y(x)$ the solution at x of the initial value problem (3).

The basic idea of multi-revolution Runge-Kutta (MRRK) methods is to approximate $\varphi^N(y_0)$ by using s ($s \ll N$) evaluations of φ at some suitable points $Y_j \in U$ ($j = 1, \ldots, s$). Evidently, the case $s \geq N$ is not of interest. The approximation y_N to $\varphi^N(y_0)$ by an s-stage *multi-revolution Runge-Kutta (MRRK) method* is defined by the equations

$$Y_i = y_0 + N \sum_{j=1}^{s} a_{ij}(\varphi(Y_j) - Y_j), \quad \text{for } i = 1, \ldots, s, \tag{4a}$$

$$y_N = y_0 + N \sum_{i=1}^{s} b_i(\varphi(Y_i) - Y_i), \tag{4b}$$

where $b = (b_i) \in \mathbb{R}^s$ and $A = (a_{ij}) \in \mathbb{R}^{s\times s}$ are real coefficients (that may depend on N) which define the MRRK algorithm. We stress the fact that in practice MRRK methods do not depend on any small parameter ε, as can be observed from the above definition, but as the theoretical assumption (2) might misleadingly suggest. Using the theoretical assumption (2) MRRK methods can be rewritten equivalently as standard RK methods applied to (3) with the same coefficients (A, b)

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j), \quad \text{for } i = 1, \dots, s, \tag{5a}$$

$$y_N = y_0 + h\sum_{i=1}^{s} b_i f(Y_i), \tag{5b}$$

and where $h := \varepsilon N$ plays the formal role of a "stepsize". We assume existence and uniqueness in U to the implicit equations (4a) which define the values Y_i for $i = 1, \dots, s$, e.g., by having h sufficiently small. To represent the MRRK coefficients, it is natural to use a Butcher-tableau notation

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \quad \equiv \quad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

where $c = (c_i) \in \mathbb{R}^s$ are related coefficients generally satisfying $c_i = \sum_{j=1}^{s} a_{ij}$ for $i = 1, \dots, s$. Clearly if $a_{ij} = 0$ for all $j \geq i$ the method is explicit and its practical application requires s evaluations of the map φ. Here, we will consider general (i.e., implicit) methods for which A is not necessarily lower triangular.

MRRK methods aim at approximating $\varphi^N(y_0)$. The expression $\varphi^N(y_0)$ can also be interpreted as the application to (3) of one step with "stepsize" $h := \varepsilon N$ of an N-stage explicit RK method with coefficients given by the Butcher-tableau

$$\begin{array}{c|c} \mu & \Lambda \\ \hline & \beta^T \end{array}$$

with $\Lambda = (\lambda_{ij}) \in \mathbb{R}^{N\times N}$, $\beta = (\beta_i) \in \mathbb{R}^N$, and $\mu = (\mu_i) \in \mathbb{R}^N$ given as follows

$$\lambda_{ij} := \begin{cases} 1/N & \text{for } 1 \leq j < i \leq N, \\ 0 & \text{for } 1 \leq i \leq j \leq N, \end{cases} \tag{6a}$$

$$\beta_i := \frac{1}{N}, \qquad \mu_i := \sum_{j=1}^{N} \lambda_{ij} = \frac{i-1}{N} \quad \text{for } i = 1, \dots, N. \tag{6b}$$

Of course, $\varphi^N(y_0)$ can also be interpreted as an N-stage MRRK method (4) with such coefficients.

By using the rooted tree theory developed by Butcher [1,2] and Hairer et al. [8] we can expand the exact value $\varphi^N(y_0)$ and the MRRK approximation y_N as Taylor B-series in powers of $h := \varepsilon N$ as follows

$$\varphi^N(y_0) = y_0 + \sum_{q=1}^{Q} \frac{h^q}{q!} \sum_{t\in T_q} \alpha(t)\gamma(t) \left(\sum_{i=1}^{N} \beta_i \Phi_i^{\Lambda}(t) \right) F(t)(y_0) + \mathcal{O}(h^{Q+1}), \tag{7}$$

$$y_N = y_0 + \sum_{q=1}^{Q} \frac{h^q}{q!} \sum_{t\in T_q} \alpha(t)\gamma(t) \left(\sum_{i=1}^{s} b_i \Phi_i^{A}(t) \right) F(t)(y_0) + \mathcal{O}(h^{Q+1}). \tag{8}$$

Notice that these series are asymptotic series and they do not converge in general when $Q \to \infty$. The order $\rho(t)$ of a tree t is the number of its nodes. The set T_q is the set of trees t of order $\rho(t) = q$, $\alpha(t)$ and $\gamma(t)$ are real functions defined on the trees $t \in \cup_{q\geq 1} T_q$, $F(t)(y_0) \in \mathbb{R}^m$ is the elementary differential of f associated to the tree t and evaluated at the point $y_0 \in \mathbb{R}^m$. For any square matrix $\Theta = (\theta_{ij}) \in \mathbb{R}^{d\times d}$, the vector function $\Phi^{\Theta} : \cup_{q\geq 1} T_q \to \mathbb{R}^d$ with components Φ_i^{Θ} $(i = 1, \ldots, d)$ is defined recursively by

a) $\Phi_i^{\Theta}(\tau) = 1$ for the only tree τ of order $\rho(\tau) = 1$;
b) For $t = [t_1, \ldots, t_n]$

$$\Phi_i^{\Theta}(t) = \sum_{j_1=1}^{d} \cdots \sum_{j_n=1}^{d} \theta_{ij_1} \cdots \theta_{ij_n} \Phi_{j_1}^{\Theta}(t_1) \cdots \Phi_{j_n}^{\Theta}(t_n).$$

The *order* of an MRRK method is defined as the largest integer value κ such that the coefficients of all elementary differentials in (7) and (8) are identical for all trees t of order $\rho(t) \leq \kappa$, i.e.,

$$\sum_{i=1}^{s} b_i \Phi_i^{A}(t) = \sum_{i=1}^{N} \beta_i \Phi_i^{\Lambda}(t) \quad \text{for all trees } t,\ \rho(t) \leq \kappa.$$

From Lemma 1 and Remark 1 the order conditions of MRRK methods for $N \to \infty$ converge to the order conditions of RK methods for the solution of (3). Therefore, if the coefficients of an MRRK method of order κ converge for $N \to \infty$, they must converge to the coefficients of an RK method of order κ. The asymptotic series (7) and (8) are in good agreement when $h := \varepsilon N$ is small. Therefore, in practical applications the choice of N depends on the size of $h := \varepsilon N$, more precisely it depends on the size of the perturbation $\varphi(y) - y = \varepsilon f(y)$ in (2) and of its derivatives. Observe that for periodic

orbits of exact period T we have $\epsilon = 0$ and therefore any MRRK method is exact as long as the period T is known exactly. Hence, for periodic orbits the major problem is actually to compute the period T exactly if one wants to obtain the exact solution after zillions of revolutions!

3 Simplifying assumptions and order estimates

Now we turn our attention to the analysis of the order conditions. We adopt the convention that $0^0 = 1$. The simplifying assumptions $B_N(p)$, $C_N(q)$, $D_N(r)$ below are motivated by the following lemma:

Lemma 1 *The coefficients* (Λ, β, μ) *of (6) satisfy the relations*

$$\text{(9a)} \qquad \sum_{i=1}^{N} \beta_i \mu_i^{k-1} = \delta(k, N) \quad \text{for } k = 1, 2, \ldots$$

$$\sum_{j=1}^{N} \lambda_{ij} \mu_j^{k-1} = \sum_{l=0}^{k} \rho_l(k, N) \mu_i^l$$

$$\text{(9b)} \qquad \text{for } i = 1, \ldots, N, \text{ and } k = 1, 2, \ldots$$

$$\sum_{i=1}^{N} \beta_i \mu_i^{k-1} \lambda_{ij} = \beta_j \sum_{l=0}^{k} \sigma_l(k, N) \mu_j^l$$

$$\text{(9c)} \qquad \text{for } j = 1, \ldots, N, \text{ and } k = 1, 2, \ldots$$

where explicit expressions for the scalar coefficients $\delta(k, N)$, $\rho_l(k, N)$, $\sigma_l(k, N)$ $(0 \le l \le k)$ *are given in terms of the Bernoulli numbers* B_i *as follows*

$$\rho_l(k, N) = \begin{cases} 0 & \text{for } l = 0, \\ \dfrac{1}{k}\binom{k}{l}\dfrac{B_{k-l}}{N^{k-l}} & \text{for } l = 1, 2, \ldots, k, \end{cases}$$

$$\delta(k, N) = \sum_{l=0}^{k} \rho_l(k, N) = \frac{1}{k} \sum_{l=1}^{k} \binom{k}{l} \frac{B_{k-l}}{N^{k-l}},$$

$$\sigma_0(1, N) = 1 - \frac{1}{N}, \quad \sigma_1(1, N) = -1,$$

$$\text{for } k \ge 2: \quad \sigma_l(k, N) = \begin{cases} \delta(k, N) & \text{for } l = 0, \\ \rho_l(k, N) & \text{for } l = k - 1, \\ -\rho_l(k, N) & \text{for } l \ne 0, k - 1. \end{cases}$$

Proof. The proof is based on the identity

$$\sum_{j=1}^{n}(j-1)^{k-1} = \frac{1}{k}\sum_{l=1}^{k}\binom{k}{l}B_{k-l}n^l$$

valid for $n = 1, 2, \ldots$ and $k = 1, 2, \ldots$ □

For a given s-stage MRRK method with coefficients (A, b, c) we introduce the simplifying assumptions

$$B_N(p): \quad \sum_{i=1}^{s} b_i c_i^{m-1} = \delta(m, N) \quad \text{for } m = 1, \ldots, p,$$

$$C_N(q): \quad \sum_{j=1}^{s} a_{ij} c_j^{m-1} = \sum_{l=0}^{m} \rho_l(m, N) c_i^l \quad \text{for } i = 1, \ldots, s, \text{ and } m = 1, \ldots, q,$$

$$D_N(r): \quad \sum_{i=1}^{s} b_i c_i^{m-1} a_{ij} = b_j \sum_{l=0}^{m} \sigma_l(m, N) c_j^l \quad \text{for } j = 1, \ldots, s, \text{ and } m = 1, \ldots, r.$$

Remark 1

- From Lemma 1 when $N \to \infty$ these simplifying assumptions reduce to the usual simplifying assumptions $B(p)$, $C(q)$, and $D(r)$ [1,2,8] since

  $\lim_{N\to\infty} \rho_l(k, N) = 0 \quad$ for $l = 0, 1, 2, \ldots, k-1$,

  $\lim_{N\to\infty} \sigma_l(k, N) = 0 \quad$ for $l = 1, 2, \ldots, k-1$,

  $\lim_{N\to\infty} \sigma_0(k, N) = \lim_{N\to\infty} \delta(k, N) = \lim_{N\to\infty} \rho_k(k, N) = \frac{1}{k}$,

  $\lim_{N\to\infty} \sigma_k(k, N) = -\frac{1}{k}$.

- The relations (9) imply that for $s = N$ the coefficients (Λ, β, μ) satisfy the conditions $B_N(\infty)$, $C_N(\infty)$, and $D_N(\infty)$, i.e., $B_N(p)$, $C_N(q)$, and $D_N(r)$ for all $p, q, r \geq 1$.

Some necessary conditions for the simplifying assumptions are given in the next theorem:

Theorem 1 *Assume that the MRRK coefficients (A, b, c) satisfy $b_i \neq 0$ for $i = 1, \ldots, s$ and $c_i \neq c_j$ for $i, j = 1, \ldots, s$. Then:*

- *If $B_N(s + q)$ and $D_N(s)$ hold then $C_N(q)$ must hold;*
- *If $B_N(s + r)$ and $C_N(s)$ hold then $D_N(r)$ must hold;*
- *If the MRRK method is of order $s + k$ then $C_N(k)$ and $D_N(k)$ must hold;*
- *If the MRRK method is of order $2s - 3$ then $C_N(s - 2)$ must hold.*

Proof. Let

$$d_i^{(m)} := \sum_{j=1}^{s} a_{ij} c_j^{m-1} - \sum_{l=0}^{m} \rho_l(m, N) c_i^l \quad \text{for } i = 1, \dots, s, \text{ and } m = 1, \dots, q.$$

$C_N(q)$ is equivalent to $d_i^{(m)} = 0$ for $i = 1, \dots, s$, and $m = 1, \dots, q$. We have under $B_N(s+q)$ and $D_N(s)$

$$\sum_{i=1}^{s} b_i c_i^{k-1} d_i^{(m)} = \sum_{l=0}^{k} \sigma_l(k, N) \delta(l+m, N) - \sum_{l=0}^{m} \rho_l(m, N) \delta(l+k, N). \tag{10}$$

for $k = 1, \dots, s$. The right-hand side is an expression which is independent of the MRRK coefficients, in particular of s. There exist MRRK methods with S stages satisfying $B_N(s+q)$, $D_N(s)$, and $C_N(q)$. For $k = 1, \dots, s$ these methods also satisfy the above equality (10) with s replaced by S. Moreover, the left-hand side of (10) vanishes for those methods. For example, one can take the N-stage MRRK method with coefficients (Λ, β, μ) which satisfies $B_N(\infty)$, $C_N(\infty)$, and $D_N(\infty)$. Hence, the sum on the right-hand side of (11) must be equal to zero. Therefore, for the original MRRK coefficients considered we have $d_i^{(m)} = 0$ for $i = 1, \dots, s$ since $(c_i^{k-1})_{i,k=1}^{s}$ is an invertible Vandermonde matrix and $b_i \neq 0$ for $i = 1, \dots, s$.

Similarly, for the second statement, let

$$d_j^{(m)} := \sum_{i=1}^{s} b_i c_i^{m-1} a_{ij} - b_j \sum_{l=0}^{m} \sigma_l(m, N)\, c_j^l \quad \text{for } j = 1, \dots, s, \text{ and } m = 1, \dots, r.$$

$D_N(r)$ is equivalent to $d_j^{(m)} = 0$ for $j = 1, \dots, s$, and $m = 1, \dots, r$. We have under $B_N(s+r)$ and $C_N(s)$

$$\sum_{j=1}^{s} d_j^{(m)} c_j^{k-1} = \sum_{l=0}^{k} \rho_l(k, N)\, \delta(l+m, N) - \sum_{l=0}^{m} \sigma_l(m, N)\, \delta(l+k, N) \tag{11}$$

for $k = 1, \dots, s$. The right-hand side is again an expression which is independent of the MRRK coefficients, in particular of s. There exist MRRK methods with S stages satisfying $B_N(s+r)$, $C_N(s)$, and $D_N(r)$. For $k = 1, \dots, s$ these

methods also satisfy the above equality (11) with s replaced by S. Moreover, the left-hand side of (11) vanishes for those methods. For example, one can take the N-stage MRRK method with coefficients (Λ, β, μ) which satisfies $B_N(\infty)$, $C_N(\infty)$, and $D_N(\infty)$. Hence, the sum on the right-hand side of (11) must be equal to zero. Therefore, for the original MRRK coefficients considered we have $d_j^{(m)} = 0$ for $j = 1, \ldots, s$ since $(c_j^{k-1})_{j,k=1}^{s}$ is an invertible Vandermonde matrix.

The proof of the third statement is totally similar to the above proofs, see also [15]. The proof of the fourth statement can be made similarly to the one given in [15, Proposition 2.8], hence we omit it. □

Remark 2 As long as relations of the type (9) are satisfied, the proof given above is fairly general and completely independent of the values of the coefficients $\delta(k, N)$, $\rho_l(k, N)$, and $\sigma_l(k, N)$ for $l = 0, \ldots, k$.

We can prove a result similar to a famous one due to Butcher [1,2,8]:

Theorem 2 *If $B_N(p)$, $C_N(q)$, and $D_N(r)$ are satisfied then the MRRK method (4) is at least of order $\kappa = \min(p, 2q + 2, q + r + 1)$.*

Proof. Assuming

$$\sum_{i=1}^{s}\sum_{j=1}^{s} b_i \Phi_{ij}^{A} c_j^{l} = \sum_{i=1}^{N}\sum_{j=1}^{N} \beta_i \Phi_{ij}^{\Lambda} \mu_j^{l} \quad \text{for } l = 0, \ldots, q, \tag{12}$$

we obtain for $1 \le m \le q$

$$\begin{aligned}
\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} b_i \Phi_{ij}^{A} a_{jk} c_k^{m-1} &= \sum_{i=1}^{s}\sum_{j=1}^{s} b_i \Phi_{ij}^{A} \left(\sum_{l=0}^{m} \rho_l(m, N) c_j^{l} \right) \\
&= \sum_{l=0}^{m} \rho_l(m, N) \left(\sum_{i=1}^{N}\sum_{j=1}^{N} \beta_i \Phi_{ij}^{\Lambda} \mu_j^{l} \right) \\
&= \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N} \beta_i \Phi_{ij}^{\Lambda} \lambda_{jk} \mu_k^{m-1}
\end{aligned}$$

where we have used successively $C_N(q)$, the assumption (12), and the property (9b). That implies for $u_1, \ldots, u_n$ arbitrary sub-trees, we can reduce the order conditions of a tree t containing a sub-tree of the form $[u_1, \ldots, u_n, [\tau^1, \ldots, \tau^{m-1}]]$ to the order conditions of trees as t, but with this sub-tree being replaced by $[u_1, \ldots, u_n, \tau^1, \ldots, \tau^l]$ for $l = 0, \ldots, m$.

Assuming

$$\sum_{j=1}^{s} b_j c_j^{l} \Phi_j^{A} = \sum_{j=1}^{N} \beta_j \mu_j^{l} \Phi_j^{\Lambda} \quad \text{for } l = 0, \ldots, r, \tag{13}$$

we obtain for $1 \le m \le r$

$$\sum_{i=1}^{s}\sum_{j=1}^{s} b_i c_i^{m-1} a_{ij} \Phi_j^A = \sum_{j=1}^{s} b_j \left(\sum_{l=0}^{m} \sigma_l(m, N) c_j^l \right) \Phi_j^A$$
$$= \sum_{l=0}^{m} \sigma_l(m, N) \left(\sum_{j=1}^{N} \beta_j \mu_j^l \Phi_j^\Lambda \right)$$
$$= \sum_{i=1}^{N}\sum_{j=1}^{N} \beta_i \mu_i^{m-1} \lambda_{ij} \Phi_j^\Lambda$$

where we have used successively $D_N(r)$, the assumption (13), and the property (9c). That implies for u an arbitrary sub-tree, we can reduce the order conditions of a tree t of the form $[\tau^1, \ldots, \tau^{m-1}, [u]]$ to the order conditions of trees of the form $[\tau^1, \ldots, \tau^l, u]$ for $l = 0, \ldots, m$.

We have now reduced the order conditions to the bushy trees with less than κ nodes. They are satisfied by assumption $B_N(p)$. □

Remark 3 Once again as long as relations of the type (9) are satisfied, the proof given above is independent of the specific values of the coefficients $\delta(k, N)$, $\rho_l(k, N)$, and $\sigma_l(k, N)$ for $l = 0, \ldots, k$.

4 Preservation of geometric properties

The study of numerical methods for differential equations that preserve some geometric properties of the flow has been the subject of an extensive bibliography in the last few decades. As a matter of fact, the recent book of Hairer, Lubich, and Wanner [7] provides a unified presentation of the subject pointing out why geometric integrators play a crucial role when one is interested in numerical solutions that preserve the qualitative behavior of the flow of the original model or else in long-term integrations. In the following two subsections we characterize MRRK methods preserving constant Poisson/symplectic structures and reversibility properties. The first one is associated to the flow map of Poisson/Hamiltonian systems that describe many non dissipative dynamical systems, whereas the second one is associated for example to the reversibility of the flow map of conservative mechanical systems.

4.1 Poisson/symplectic MRRK methods

We consider a skew-symmetric matrix function $J : \mathbb{R}^m \longrightarrow \mathbb{R}^{m\times m}$ satisfying the Jacobi identity

$$\sum_{l=1}^{m} \left(\frac{\partial J_{ij}(y)}{\partial y_l} J_{lk}(y) + \frac{\partial J_{jk}(y)}{\partial y_l} J_{li}(y) + \frac{\partial J_{ki}(y)}{\partial y_l} J_{lj}(y) \right) = 0$$

for $i, j, k = 1, \ldots, m$. The matrix function $J(y)$ is called a *Poisson tensor*. A transformation $\varphi : \mathbb{R}^m \longrightarrow \mathbb{R}^{m\times m}$ is *Poisson* when

$$\varphi_y(y) J(y) \varphi_y^T(y) = J(\varphi(y)). \tag{14}$$

By induction, it can be verified that φ^N is also a Poisson transformation. It can be shown that for a *Hamiltonian system* of ordinary differential equations $y' = J(y) H_y^T(y)$ with $J(y)$ a Poisson tensor, the associated flow $\varphi_t(y(s)) := y(s+t)$ is Poisson provided $J(y)$ and $H(y)$ are sufficiently smooth [13].

We want to characterize MRRK methods preserving the Poisson structure (14) for φ^N, i.e. MRRK satisfying

$$\left(\frac{\partial y_N(y_0)}{\partial y_0}\right) J(y_0) \left(\frac{\partial y_N(y_0)}{\partial y_0}\right)^T = J(y_N(y_0)). \tag{15}$$

Such methods will be called *Poisson/symplectic*. We can show the following result.

Theorem 3 *For a constant Poisson tensor J, the Poisson structure (14) for φ^N is preserved by MRRK methods satisfying $m_{ij} = 0$ for $i, j = 1, \ldots, s$ where*

$$m_{ij} := b_i a_{ij} + b_j a_{ji} - b_i b_j + \frac{1}{N} b_i \delta_{ij} \tag{16}$$

and δ_{ij} is the Kronecker-delta symbol.

Proof. To simplify the notation in this proof, we do not express explicitly the dependence of $y_N = y_N(y_0)$ and $Y_i = Y_i(y_0)$ for $i = 1, \ldots, s$ on y_0. We first assume the Poisson tensor J to be regular. Instead of trying to verify (15) directly, we can show equivalently that the condition

$$\left(\frac{\partial y_N}{\partial y_0}\right)^T J^{-1} \left(\frac{\partial y_N}{\partial y_0}\right) = J^{-1}$$

is satisfied. This condition turns out to be relatively easy to check, whereas, by using similar techniques, the condition (15) seems difficult to show directly. From (2) and (5) we have

$$\begin{aligned} \frac{\partial y_N}{\partial y_0} &= I + h \sum_{i=1}^{s} b_i \left(\frac{\partial f(Y_i)}{\partial y_0}\right), \\ \frac{\partial Y_i}{\partial y_0} &= I + h \sum_{j=1}^{s} a_{ij} \left(\frac{\partial f(Y_j)}{\partial y_0}\right) \end{aligned} \tag{17}$$

where we have defined $h := \varepsilon N$. We compute

$$
\begin{aligned}
Q &:= \left(\frac{\partial y_N}{\partial y_0}\right)^T J^{-1} \left(\frac{\partial y_N}{\partial y_0}\right) \\
&= J^{-1} + h \sum_{i=1}^{s} b_i \left(\frac{\partial f(Y_i)}{\partial y_0}\right)^T J^{-1} I + h \sum_{j=1}^{s} b_j I^T J^{-1} \left(\frac{\partial f(Y_j)}{\partial y_0}\right) \\
&\quad + h^2 \sum_{i,j=1}^{s} b_i b_j \left(\frac{\partial f(Y_i)}{\partial y_0}\right)^T J^{-1} \left(\frac{\partial f(Y_j)}{\partial y_0}\right)
\end{aligned}
$$

where we have introduced two identity matrices I and I^T. We can replace them by the following expressions coming from the second equality in (17)

$$
\begin{aligned}
I &= \left(\frac{\partial Y_i}{\partial y_0}\right) - h \sum_{j=1}^{s} a_{ij} \left(\frac{\partial f(Y_j)}{\partial y_0}\right), \\
I^T &= \left(\frac{\partial Y_j}{\partial y_0}\right)^T - h \sum_{i=1}^{s} a_{ji} \left(\frac{\partial f(Y_i)}{\partial y_0}\right)^T,
\end{aligned}
$$

and we obtain the following expression

$$
\begin{aligned}
Q = J^{-1} &+ h \sum_{i=1}^{s} b_i \left(\frac{\partial Y_i}{\partial y_0}\right)^T \left(f_y^T(Y_i) J^{-1} + J^{-1} f_y(Y_i)\right) \left(\frac{\partial Y_i}{\partial y_0}\right) \\
&+ h^2 \sum_{i,j=1}^{s} \left(b_i b_j - b_i a_{ij} - b_j a_{ji}\right) \left(\frac{\partial f(Y_i)}{\partial y_0}\right)^T J^{-1} \left(\frac{\partial f(Y_j)}{\partial y_0}\right).
\end{aligned}
$$

From $\varphi(y) = y + \varepsilon f(y)$ and (14) for φ we have

$$
f_y^T(y) J^{-1} + J^{-1} f_y(y) = -\varepsilon f_y^T(y) J^{-1} f_y(y).
$$

Hence, we finally obtain

$$
Q = J^{-1} - h^2 \sum_{i,j=1}^{s} m_{ij} \left(\frac{\partial f(Y_i)}{\partial y_0}\right)^T J^{-1} \left(\frac{\partial f(Y_j)}{\partial y_0}\right).
$$

Under the assumption $m_{ij} = 0$ for $i, j = 1, \ldots, s$ the last term vanishes. Hence, $Q = J^{-1}$ and this concludes the proof when the Poisson tensor J is regular.

When the Poisson tensor J is singular, since J is skew-symmetric, there exists an orthogonal matrix U such that

$$
U J U^T = \begin{pmatrix} \widetilde{J} & O \\ O & O \end{pmatrix}
$$

with $\widetilde{J}$ skew-symmetric and regular. In the new coordinates $z = (v^T, w^T)^T := Uy$ we have for $\phi(z) := \varphi(U^T z)$

$$\left(\frac{\partial \phi(z)}{\partial v}\right) \widetilde{J} \left(\frac{\partial \phi(z)}{\partial v}\right)^T = \widetilde{J}. \tag{18}$$

MRRK methods are invariant under linear changes of coordinates, hence the condition (15) is equivalent to

$$\left(\frac{\partial v_N}{\partial v_0}\right) \widetilde{J} \left(\frac{\partial v_N}{\partial v_0}\right)^T = \widetilde{J}$$

which must hold from the first part of the proof. □

4.2 Reversibility and symmetries of MRRK methods

A transformation φ is σ*-reversible* when

$$\sigma \circ \varphi = \varphi^{-1} \circ \sigma. \tag{19}$$

By induction, we easily find that φ^N is also σ-reversible, i.e.,

$$\sigma \circ \varphi^N = \varphi^{-N} \circ \sigma.$$

To simplify the presentation we denote the application of an MRRK method (4) by $\Psi_{\varphi,N}$, so that $\Psi_{\varphi,N}(y_0) = y_N$. We recall that $\Psi_{\varphi,N}$ aims at approximating φ^N. A multi-revolution method is σ-reversible if

$$\sigma \circ \Psi_{\varphi,N} = \left(\Psi_{\varphi,N}\right)^{-1} \circ \sigma. \tag{20}$$

We would like to characterize MRRK methods which are σ-reversible. For example, we trivially have that $\Psi_{\varphi,N} := \varphi^N$ is σ-reversible. When σ is linear, MRRK methods have the property

$$\sigma \circ \Psi_{\varphi,N} = \Psi_{\varphi^{-1},N} \circ \sigma,$$

since from (4) and (19) we have

$$\sigma Y_i = \sigma y_0 + N \sum_{j=1}^{s} a_{ij} (\varphi^{-1}(\sigma Y_j) - \sigma Y_j) \quad \text{for } i = 1, \ldots, s,$$

$$\sigma y_N = \sigma y_0 + N \sum_{i=1}^{s} b_i (\varphi^{-1}(\sigma Y_i) - \sigma Y_i).$$

We define *(φ^{-1})-symmetric* MRRK methods those which satisfy $\Psi_{\varphi^{-1},N} = (\Psi_{\varphi,N})^{-1}$ or equivalently

$$\left(\Psi_{\varphi^{-1},N}\right)^{-1} = \Psi_{\varphi,N}. \tag{21}$$

Hence, when σ is linear an MRRK method is σ-reversible if and only if it is (φ^{-1})-symmetric. Another possible definition of symmetry is to define *$(-N)$-symmetric* MRRK methods those which satisfy $\Psi_{\varphi,-N} = (\Psi_{\varphi,N})^{-1}$ or equivalently $(\Psi_{\varphi,-N})^{-1} = \Psi_{\varphi,N}$. However, this kind of symmetry is not relevant concerning the preservation of σ-reversibility. Nevertheless, notice that φ^N, which can be interpreted as an MRRK method, is trivially both (φ^{-1})-symmetric and $(-N)$-symmetric. In the following theorem we give sufficient conditions for the (φ^{-1})-symmetry of MRRK methods, hence for their σ-reversibility.

Theorem 4 *If the coefficients of an MRRK method satisfy*

$$a_{ij} + a_{s+1-i,s+1-j} + \frac{\delta_{ij}}{N} = b_j = b_{s+1-j} \quad \text{for } i, j = 1, \dots, s, \tag{22}$$

where δ_{ij} is the Kronecker-delta symbol, then the MRRK method is (φ^{-1})-symmetric, i.e., (21) is satisfied.

Proof. The expression of $\widehat{y}_N := \Psi_{\varphi^{-1},N}(y_0)$ is as follows

$$\widehat{Y}_i = y_0 + N \sum_{j=1}^{s} a_{ij}(\varphi^{-1}(\widehat{Y}_j) - \widehat{Y}_j) \quad \text{for } i = 1, \dots, s,$$

$$\widehat{y}_N = y_0 + N \sum_{i=1}^{s} b_i(\varphi^{-1}(\widehat{Y}_i) - \widehat{Y}_i).$$

We want to express the corresponding MRRK method in terms of φ. We define $\widehat{Z}_j := \varphi^{-1}(\widehat{Y}_j)$ and we obtain the relation

$$\varphi(\widehat{Z}_i) = y_0 + N \sum_{j=1}^{s} a_{ij}(\widehat{Z}_j - \varphi(\widehat{Z}_j)) \quad \text{for } i = 1, \dots, s,$$

leading to

$$\widehat{Z}_i = y_0 - N \sum_{j=1}^{s} (a_{ij} + \frac{\delta_{ij}}{N})(\varphi(\widehat{Z}_j) - \widehat{Z}_j), \quad 1 \le i \le s, \tag{23a}$$

$$\widehat{y}_N = y_0 - N \sum_{i=1}^{s} b_i(\varphi(\widehat{Z}_i) - \widehat{Z}_i). \tag{23b}$$

Now, to obtain an expression for $y_N^* := (\Psi_{\varphi^{-1},N})^{-1}(y_0)$ we simply exchange the role of y_0 and $\widehat{y}_N$ in (23). This leads to

$$Y_i^* = y_0 + N \sum_{j=1}^{s} (b_j - a_{ij} - \frac{\delta_{ij}}{N})(\varphi(Y_j^*) - Y_j^*), \ 1 \le i \le s, \tag{24a}$$

$$y_N^* = y_0 + N \sum_{i=1}^{s} b_i(\varphi(Y_i^*) - Y_i^*). \tag{24b}$$

We have obtained the *(φ^{-1})-adjoint method* to (4). (φ^{-1})-symmetric MRRK methods satisfy $y_N^* = y_N$. By reordering the internal stages Y_i in (4) such that $Y_i^* = Y_{s+1-i}$ for $i = 1, \ldots, s$, the conditions (22) are sufficient for (φ^{-1})-symmetry. □

5 Orthogonal polynomials and high order implicit MRRK methods

Our next task is to choose the nodes $c_1, \ldots, c_s$ and the weights $b_1, \ldots, b_s$ so that $B_N(p)$ holds with $p \geq s$. To this end we introduce on the set of functions $F := \{f : [0, 1] \to \mathbb{R}\}$ a discrete semi-scalar product defined for $u, v \in F$ by

$$\langle u, v \rangle := \frac{1}{N} \sum_{j=1}^{N} u\left(\frac{j-1}{N}\right) v\left(\frac{j-1}{N}\right).$$

This inner product is also a scalar product on the set of polynomials of degree $\leq N - 1$. Using this inner product, the condition $B_N(p)$ can be expressed in the form

$$B_N(p) \; : \quad \sum_{i=1}^{s} b_i c_i^{m-1} = \langle 1, x^{m-1} \rangle \quad \text{for } m = 1, \ldots, p.$$

We consider some nodes $c_1, \ldots, c_s$ and weights $b_1, \ldots, b_s$ satisfying $B_N(s)$. It is well-known that $B_N(s + k)$ for $k \geq 0$ is satisfied if and only if the nodal polynomial

$$P(x) := \prod_{j=1}^{s} (x - c_j) = (x - c_1) \cdots (x - c_s)$$

is orthogonal to all polynomials $q(x)$ with $\deg(q(x)) \leq k - 1$, and that the maximal possible value of $s+k$ is equal to $2s$. This motivates the construction of a family of orthogonal polynomials. Starting with $P_0(x) := 1$, we denote by $P_n(x) = x^n + Q_n(x)$ with $\deg(Q_n(x)) \leq n - 1$ for $n = 1, 2, \ldots$, the family of polynomials which are orthogonal with respect to the above inner product. It is well-known that these orthogonal polynomials exist, are unique, and satisfy a three-term recursion (with $P_{-1}(x) := 0$)

$$P_{n+1}(x) = (x - \alpha_{n+1}) P_n(x) - \beta_{n+1} P_{n-1}(x), \quad \text{for } n = 0, 1, 2, \ldots$$

with coefficients α_{n+1} and β_{n+1} (with arbitrary β_1) given by

$$\alpha_{n+1} = \frac{\langle x P_n, P_n \rangle}{\langle P_n, P_n \rangle}, \quad \beta_{n+1} = \frac{\langle P_n, P_n \rangle}{\langle P_{n-1}, P_{n-1} \rangle} \quad (n \geq 1).$$

For example we have

$$P_1(x) = x - \frac{1}{2} + \frac{1}{2N},\ P_2(x) = x^2 + \left(-1 + \frac{1}{N}\right)x + \left(\frac{1}{6} - \frac{1}{2N} + \frac{1}{3N^2}\right),$$

etc. Further, all n roots of $P_n(x)$ are real, distinct, and in the interval $[0, 1]$. Defining the discrete forward difference operator $\Delta_N f(x) := N(f(x + 1/N) - f(x))$, these orthogonal polynomials satisfy a *discrete Rodrigues' formula*

$$P_n(x) = C_{N,n}\Delta_N^n\left[\binom{xN}{n}\binom{(x-1)N}{n}\right], \quad \text{for } n = 0, 1, 2, \ldots$$

for some suitable constants $C_{N,n}$. These polynomials are also associated to distributions of Stieltjes type, see more details in [19]. The orthogonal polynomials $P_n(x)$ are symmetric with respect to the point $\zeta_N := 1/2 - 1/(2N)$. The shifted polynomials $p_n(x) := P_n(\zeta_N + x)$ are odd when n is odd and even when n is even. Simpler expressions for the shifted polynomials $p_n(x)$ than for $P_n(x)$ are obtained

$$p_0(x) = 1,\ p_1(x) = x,\ p_2(x) = x^2 - \left(\tfrac{1}{12} - \tfrac{1}{12N^2}\right),$$
$$p_3(x) = x^3 - x\left(\tfrac{3}{20} - \tfrac{7}{20N^2}\right),$$
$$p_4(x) = x^4 - x^2\left(\tfrac{3}{14} - \tfrac{13}{14N^2}\right) + \left(\tfrac{3}{560} - \tfrac{3}{56N^2} + \tfrac{27}{560N^4}\right),$$

etc. These expressions are more convenient for example to obtain explicitly the roots of $P(x)$ as below for low degrees s. Considering some weights $b_1, \ldots, b_s$ and nodes $c_1, \ldots, c_s$ satisfying $B_N(s)$, it is also well-known that $B_N(2s - k)$ is satisfied with $0 \le k \le s$ if and only if the nodes $c_1, \ldots, c_s$ are the roots of

$$P(x) := P_s(x) + \sum_{l=1}^{k} \rho_l P_{s-l}(x)$$

for some real numbers $\rho_1, \ldots, \rho_k \neq 0$.

We assume now that the nodes $c_1, \ldots, c_s$ have been fixed to some distinct values. There are different ways of obtaining the weights $b_1, \ldots, b_s$ such that $B_N(s)$ is satisfied. They can be uniquely determined by solving the system of linear equations corresponding to $B_N(s)$ with Vandermonde matrix $(c_i^{j-1})_{i,j=1}^s$. An alternative is given by

$$b_i = \langle 1, \ell_i(x)\rangle \quad \text{for } i = 1, \ldots, s$$

Table 1. Coefficients of the s-stage Gauss MRRK methods of order $2s$ ($s = 1, 2$)

$$\begin{array}{c|c} \frac{1}{2} - \frac{1}{2N} & \frac{1}{2} - \frac{1}{2N} \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} \frac{1}{2} - \frac{1}{2N} - \frac{\sqrt{3}}{6}\sqrt{1 - \frac{1}{N^2}} & \frac{1}{4} - \frac{1}{2N} & \frac{1}{4} - \frac{\sqrt{3}}{6}\sqrt{1 - \frac{1}{N^2}} \\ \frac{1}{2} - \frac{1}{2N} + \frac{\sqrt{3}}{6}\sqrt{1 - \frac{1}{N^2}} & \frac{1}{4} + \frac{\sqrt{3}}{6}\sqrt{1 - \frac{1}{N^2}} & \frac{1}{4} - \frac{1}{2N} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

where

$$\ell_i(x) := \prod_{\substack{k=1 \\ k \neq i}}^{s} \left(\frac{x - c_k}{c_i - c_k} \right), \qquad \text{for } i = 1, \ldots, s$$

are the Lagrange polynomials with respect to the nodes $c_1, \ldots, c_s$.

5.1 Gauss MRRK methods

The polynomial $P_s(x)$ of degree s is the unique polynomial of degree s which is orthogonal to all polynomials $q(x)$ with $\deg(q(x)) \leq s - 1$. Hence, by taking the nodes $c_1, \ldots, c_s$ as the roots of $P_s(x)$, the weights $b_1, \ldots, b_s$ such that $B_N(s)$ is satisfied, and the coefficients $(a_{ij})_{i,j=1}^{s}$ such that $C_N(s)$ holds, we obtain the unique method of order $2s$. It satisfies $B_N(2s)$, $C_N(s)$, and $D_N(s)$. We call this method the *s-stage Gauss MRRK method*. The s-stage Gauss MRRK coefficients for $s = 1, 2$ of order $2s = 2, 4$ are given in Table 1.

Observe that for $N \to \infty$ we obtain the coefficients of standard Gauss IRK methods [1,2,9,18].

Concerning the preservation of geometric properties we have the following results.

Theorem 5 *Gauss MRRK methods are Poisson/symplectic.*

Proof. The coefficients c_i for $i = 1, \ldots, s$ of Gauss MRRK methods are distinct. To prove that $m_{ij} = 0$ for $i, j = 1, \ldots, s$, we will show equivalently that

$$\sum_{i=1}^{s} \sum_{j=1}^{s} c_i^{k-1} m_{ij} c_j^{l-1} = 0 \quad \text{for } k, l = 1, \ldots, s. \tag{25}$$

From $B_N(2s)$ and $D_N(s)$ we have

$$\sum_{i=1}^{s}\sum_{j=1}^{s} c_i^{k-1} m_{ij} c_j^{l-1} = \sum_{m=0}^{k} \sigma_m(k,N)\delta(m+l,N) + \sum_{m=0}^{l} \sigma_m(l,N)\delta(m+k,N) - \delta(k,N)\delta(l,N) + \frac{1}{N}\delta(k+l-1,N). \tag{26}$$

We could have also used $B_N(2s)$ and $C_N(s)$. In both cases, the right-hand side is an expression which is independent of the Gauss MRRK coefficients, in particular of s. There exist MRRK methods with $S \geq s$ stages satisfying $B_N(2s)$, $D_N(s)$, $C_N(s)$ and $m_{ij} = 0$ for $i, j = 1, \ldots, S$. These methods also satisfy the above equality (26) for $k, l = 1, \ldots, s$ with s replaced by S. Moreover, the left-hand side of (26) vanishes for those methods. For example, one can take the N-stage MRRK method with coefficients (Λ, β, μ) which satisfies $B_N(\infty)$, $C_N(\infty)$, and $D_N(\infty)$. Hence, the sum on the right-hand side of (26) must be equal to zero. Therefore, for the Gauss MRRK coefficients we have (25). This leads to the desired conclusion $m_{ij} = 0$ for $i, j = 1, \ldots, s$ since $(c_i^{k-1})_{i,k=1}^{s}$ is an invertible Vandermonde matrix. □

Theorem 6 *Gauss MRRK methods are (φ^{-1})-symmetric.*

Proof. We can give a proof similar to the one of Theorem 5. Let

$$r_{ij} := a_{ij} + a_{s+1-i,s+1-j} + \frac{\delta_{ij}}{N} - b_j \quad \text{for } i, j = 1, \ldots, s.$$

From Theorem 5, Gauss MRRK methods are Poisson/symplectic, i.e., the coefficients of Gauss MRRK methods satisfy

$$b_i a_{ij} + b_j a_{ji} - b_i b_j + \frac{1}{N} b_i \delta_{ij} = 0 \quad \text{for } i, j = 1, \ldots, s.$$

Hence,

$$b_i r_{ij} = b_i a_{s+1-i,s+1-j} - b_j a_{ji} \quad \text{for } i, j = 1, \ldots, s.$$

To prove that $r_{ij} = 0$ for $i, j = 1, \ldots, s$ we can show equivalently that

$$\sum_{i=1}^{s}\sum_{j=1}^{s} b_i c_i^{k-1} r_{ij} c_j^{l-1} = 0 \quad \text{for } k, l = 1, \ldots, s. \tag{27}$$

Gauss MRRK coefficients satisfy $c_{s+1-i} = 1 - c_i - 1/N$ and $b_{s+1-i} = b_i$ for $i = 1, \ldots, s$. As in the proof of Theorem 3, by application of the simplifying

Table 2. Coefficients of the s-stage Radau IA MRRK methods of order $2s-1$ ($s=1,2$)

$$\begin{array}{c|c} 0 & 1-1/N \\ \hline & 1 \end{array} \qquad \begin{array}{c|cc} 0 & \frac{1}{4}\left(\frac{(1-1/N)(1-2/N)}{1-1/(2N)}\right) & -\frac{1}{4}\left(\frac{(1-1/N)(1-2/N)}{1-1/(2N)}\right) \\ \frac{2}{3}\left(1-\frac{1}{2N}\right) & \frac{1}{4}\left(\frac{1+1/N}{1-1/(2N)}\right) & \frac{5}{12}\left(\frac{(1-2/N)(1-1/(5N))}{1-1/(2N)}\right) \\ \hline & \frac{1}{4}\left(\frac{1+1/N}{1-1/(2N)}\right) & \frac{3}{4}\left(\frac{1-1/N}{1-1/(2N)}\right) \end{array}$$

assumptions $B_N(2s)$ and $D_N(s)$ we can reduce the expressions (27) to expressions independent of the Gauss MRRK coefficients, in particular of s. There exist MRRK methods with $S \geq s$ stages satisfying $B_N(2s)$, $D_N(s)$, $C_N(s)$ and $r_{ij}=0$ for $i,\, j=1,\ldots,S$. These methods satisfy the equalities (27) for $k,l=1,\ldots,s$ with s replaced by S. For example, one can take the N-stage MRRK method with coefficients (Λ,β,μ) which satisfies $B_N(\infty)$, $C_N(\infty)$, and $D_N(\infty)$. Therefore, for the Gauss MRRK coefficients we have (27). This leads to the desired conclusion $r_{ij}=0$ for $i,\, j=1,\ldots,s$ since $(c_i^{k-1})_{i,k=1}^{s}$ is an invertible Vandermonde matrix and $b_i \neq 0$ for $i=1,\ldots,s$. □

5.2 Radau IA MRRK methods

We consider the polynomials

$$P_n^I(x) := C_{N,n}^I \Delta_N^{n-1}\left[\binom{xN}{n}\binom{(x-1)N}{n-1}\right], \qquad \text{for } n=1,2,3,\ldots$$

for some normalization constants $C_{N,n}^I$. The polynomial $P_s^I(x)$ of degree $s \geq 1$ is orthogonal to all polynomials $q(x)$ with $\deg(q(x)) \leq s-2$. Moreover, $c_1=0$ is a root of $P_s^I(x)$. By taking the nodes $c_1=0,\ldots,c_s$ as the roots of $P_s^I(x)$, the weights $b_1,\ldots,b_s$ such that $B_N(s)$ is satisfied, and the coefficients $(a_{ij})_{i,j=1}^{s}$ such that $D_N(s)$ holds, we obtain a method of order $2s-1$, satisfying $B_N(2s-1)$, $C_N(s-1)$, and $D_N(s)$. We call this method the *s-stage Radau IA MRRK method*. The s-stage Radau IA MRRK coefficients for $s=1,2$ of order $2s-1=1,3$ are given in Table 2. Observe that for $N \to \infty$ we obtain the coefficients of standard Radau IA IRK methods [1, 2, 9].

5.3 Radau IIA MRRK methods

We consider the polynomials

$$P_n^{II}(x) := C_{N,n}^{II} \Delta_N^{n-1}\left[\binom{xN}{n-1}\binom{(x-1)N}{n}\right], \qquad \text{for } n=1,2,3,\ldots$$

Table 3. Coefficients of the s-stage Radau IIA MRRK methods of order $2s-1$ ($s=1,2$)

$\frac{1}{3}\left(1-\frac{1}{N}\right)$	$\frac{5}{12}\left(\frac{(1-1/N)(1+4/(5N))}{1+1/(2N)}\right)$	$-\frac{1}{12}\left(\frac{(1-1/N)(1+2/N)}{1+1/(2N)}\right)$
1	$\frac{3}{4}\left(\frac{1+1/N}{1+1/(2N)}\right)$	$\frac{1}{4}\left(\frac{1-1/N}{1+1/(2N)}\right)$
	$\frac{3}{4}\left(\frac{1+1/N}{1+1/(2N)}\right)$	$\frac{1}{4}\left(\frac{1-1/N}{1+1/(2N)}\right)$

for some normalization constants $C_{N,n}^{II}$. The polynomial $P_s^{II}(x)$ of degree $s \geq 1$ is orthogonal to all polynomials $q(x)$ with $\deg(q(x)) \leq s-2$. Moreover, $c_s = 1$ is a root of $P_s^{II}(x)$. By taking the nodes $c_1, \ldots, c_s = 1$ as the roots of $P_s^{II}(x)$, the weights $b_1, \ldots, b_s$ such that $B_N(s)$ is satisfied, and the coefficients $(a_{ij})_{i,j=1}^s$ such that $C_N(s)$ holds, we obtain a method of order $2s-1$, satisfying $B_N(2s-1)$, $C_N(s)$, and $D_N(s-1)$. We call this method the *s-stage Radau IIA MRRK method*. The s-stage Radau IIA MRRK coefficients for $s=1,2$ of order $2s-1=1,3$ are given in Table 3. Observe that for $N \to \infty$ we obtain the coefficients of standard Radau IIA IRK methods [1,2,9].

5.4 Lobatto IIIA-B-C-C-D MRRK methods*

We consider the polynomials

$$P_n^{III}(x) := C_{N,n}^{III} \Delta_N^{n-2} \left[\binom{xN}{n-1} \binom{(x-1)N}{n-1} \right], \quad \text{for } n = 2, 3, 4 \ldots$$

for some normalization constants $C_{N,n}^{III}$. The polynomial $P_s^{III}(x)$ of degree $s \geq 2$ is orthogonal to all polynomials $q(x)$ with $\deg(q(x)) \leq s-3$. Moreover, $c_1 = 0$ and $c_s = 1$ are two roots of $P_s^{III}(x)$. By taking the nodes $c_1 = 0, c_2, \ldots, c_s = 1$ as the roots of $P_s^{III}(x)$, the weights $b_1, \ldots, b_s$ such that $B_N(s)$ is satisfied, the assumption $B_N(2s-2)$ must hold. We discuss five choices for the coefficients $(a_{ij})_{i,j=1}^s$.

By taking the coefficients $(a_{ij})_{i,j=1}^s$ such that $C_N(s)$ holds, we obtain a method of order $2s-2$, satisfying $B_N(2s-2)$, $C_N(s)$, and $D_N(s-2)$. We call this method the *s-stage Lobatto IIIA MRRK method*. The s-stage Lobatto IIIA MRRK coefficients for $s=2,3$ of order $2s-2=2,4$ are given in Table 4. Observe that for $N \to \infty$ we obtain the coefficients of standard Lobatto IIIA IRK methods [1,2,9]. Similarly to Theorem 6 we can prove:

Theorem 7 *Lobatto IIIA MRRK methods are (φ^{-1})-symmetric.*

By taking the coefficients $(a_{ij})_{i,j=1}^s$ such that $D_N(s)$ holds, we obtain a method of order $2s-2$, satisfying $B_N(2s-2)$, $C_N(s-2)$, and $D_N(s)$. We

Table 4. Coefficients of the s-stage Lobatto IIIA MRRK methods of order $2s-2$ ($s = 2, 3$)

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \\ \hline & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24}+\frac{1}{2N}+\frac{1}{6N^2} & \frac{1}{3}-\frac{1}{2N}-\frac{1}{3N^2} & -\frac{1}{24}+\frac{1}{6N^2} \\ 1 & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \\ \hline & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \end{array}$$

Table 5. Coefficients of the s-stage Lobatto IIIB MRRK methods of order $2s-2$ ($s = 2, 3$)

$$\begin{array}{c|cc} 0 & \frac{1}{2}-\frac{1}{2N} & 0 \\ 1 & \frac{1}{2}+\frac{1}{2N} & -\frac{1}{N} \\ \hline & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \end{array} \qquad \begin{array}{c|ccc} 0 & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} & -\frac{1}{6}+\frac{1}{2N}-\frac{1}{3N^2} & 0 \\ \frac{1}{2} & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{1}{3}-\frac{1}{2N}-\frac{1}{3N^2} & 0 \\ 1 & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{5}{6}+\frac{1}{2N}-\frac{1}{3N^2} & -\frac{1}{N} \\ \hline & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \end{array}$$

Table 6. Coefficients of the s-stage Lobatto IIIC MRRK methods of order $2s-2$ ($s = 2, 3$)

$$\begin{array}{c|cc} 0 & \frac{1}{2}-\frac{1}{2N} & -\frac{1}{2}+\frac{1}{2N} \\ 1 & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \\ \hline & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \end{array} \qquad \begin{array}{c|ccc} 0 & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} & -\frac{1}{3}+\frac{1}{N}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \\ \frac{1}{2} & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{5}{12}-\frac{1}{2N}-\frac{2}{3N^2} & -\frac{1}{12}+\frac{1}{3N^2} \\ 1 & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \\ \hline & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \end{array}$$

call this method the *s-stage Lobatto IIIB MRRK method*. The s-stage Lobatto IIIB MRRK coefficients for $s = 2, 3$ of order $2s - 2 = 2, 4$ are given in Table 5. Observe that for $N \to \infty$ we obtain the coefficients of standard Lobatto IIIB IRK methods [1,2,9]. Similarly to Theorem 6 we can prove:

Theorem 8 *Lobatto IIIB MRRK methods are (φ^{-1})-symmetric.*

By taking the coefficients $(a_{ij})_{i,j=1}^{s}$ such that $a_{i1} = b_1 - \delta_{i1}/N$ for $i = 1, \ldots, s$ ($\delta_{i1} = 1$ if $i = 1$ else $\delta_{i1} = 0$ for $i \neq 1$) and that $C_N(s-1)$ holds, we obtain a method of order $2s - 2$, satisfying $B_N(2s-2)$, $C_N(s-1)$, and $D_N(s-1)$. We call this method the *s-stage Lobatto IIIC MRRK method*. The s-stage Lobatto IIIC MRRK coefficients for $s = 2, 3$ of order $2s - 2 = 2, 4$ are given in Table 6. Observe that for $N \to \infty$ we obtain the coefficients of standard Lobatto IIIC IRK methods [1,2,9].

Table 7. Coefficients of the s-stage Lobatto IIIC* MRRK methods of order $2s-2$ ($s=2,3$)

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1+\frac{1}{N} & -\frac{1}{N} \\ \hline & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{4}+\frac{1}{2N} & \frac{1}{4}-\frac{1}{2N} & 0 \\ 1 & 0 & 1+\frac{1}{N} & -\frac{1}{N} \\ \hline & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \end{array}$$

Table 8. Coefficients of the s-stage Lobatto IIID MRRK methods of order $2s-2$ ($s=2,3$)

$$\begin{array}{c|cc} 0 & \frac{1}{4}-\frac{1}{4N} & -\frac{1}{4}+\frac{1}{4N} \\ 1 & \frac{3}{4}+\frac{3}{4N} & \frac{1}{4}-\frac{3}{4N} \\ \hline & \frac{1}{2}+\frac{1}{2N} & \frac{1}{2}-\frac{1}{2N} \end{array} \qquad \begin{array}{c|ccc} 0 & \frac{1}{12}-\frac{1}{4N}+\frac{1}{6N^2} & -\frac{1}{6}+\frac{1}{2N}-\frac{1}{3N^2} & \frac{1}{12}-\frac{1}{4N}+\frac{1}{6N^2} \\ \frac{1}{2} & \frac{5}{24}+\frac{1}{2N}+\frac{1}{6N^2} & \frac{1}{3}-\frac{1}{2N}-\frac{1}{3N^2} & -\frac{1}{24}+\frac{1}{6N^2} \\ 1 & \frac{1}{12}+\frac{1}{4N}+\frac{1}{6N^2} & \frac{5}{6}+\frac{1}{2N}-\frac{1}{3N^2} & \frac{1}{12}-\frac{3}{4N}+\frac{1}{6N^2} \\ \hline & \frac{1}{6}+\frac{1}{2N}+\frac{1}{3N^2} & \frac{2}{3}-\frac{2}{3N^2} & \frac{1}{6}-\frac{1}{2N}+\frac{1}{3N^2} \end{array}$$

By taking the coefficients $(a_{ij})_{i,j=1}^{s}$ such that $a_{is}=-\delta_{is}/N$ for $i=1,\dots,s$ ($\delta_{is}=1$ if $i=s$ else $\delta_{is}=0$ for $i\neq s$) and that $C_N(s-1)$ holds, we obtain a method of order $2s-2$, satisfying $B_N(2s-2)$, $C_N(s-1)$, and $D_N(s-1)$. We call this method the *s-stage MRRK (Butcher's) Lobatto IIIC* method*. The s-stage Lobatto IIIC* MRRK coefficients for $s=2,3$ of order $2s-2=2,4$ are given in Table 7. Observe that for $N\to\infty$ we obtain the coefficients of standard (Butcher's) Lobatto IIIC* IRK methods [1,2,8,10].

By taking the coefficients $(a_{ij})_{i,j=1}^{s}$ such that $a_{ij}=(a_{ij}^{C}+a_{ij}^{C^*})/2$ for $i,j=1,\dots,s$ where $(a_{ij}^{C})_{i,j=1}^{s}$ are the coefficients of Lobatto IIIC methods and $(a_{ij}^{C^*})_{i,j=1}^{s}$ are the coefficients of Lobatto IIIC* methods, we obtain a method of order $2s-2$, satisfying $B_N(2s-2)$, $C_N(s-1)$, and $D_N(s-1)$. We call this method the *s-stage Lobatto IIID MRRK method*. The s-stage Lobatto IIID MRRK coefficients for $s=2,3$ of order $2s-2=2,4$ are given in Table 8. Observe that for $N\to\infty$ we obtain the coefficients of standard Lobatto IIID IRK methods [4,10]. Similarly to Theorem 5 we can prove:

Theorem 9 *Lobatto IIID MRRK methods are Poisson/symplectic.*

Similarly to Theorem 6 we can prove:

Theorem 10 *Lobatto IIID MRRK methods are (φ^{-1})-symmetric.*

6 MRRK methods for non-autonomous maps

In this section we consider the approximation of non-autonomous near identity maps, which arise in the solution of non-autonomous differential equations, by means of MRRK type algorithms.

Let $y(t, t_0, y_0)$ be the solution of a non-autonomous initial value problem

$$\frac{dy}{dt} = g(t, y), \quad y(t_0) = y_0 \in \mathbb{R}^m, \tag{28}$$

and suppose that there exist a fixed $T > 0$ and an open set $U \subset \mathbb{R}^m$ such that the map

$$\varphi_T : (t, y) \mapsto y(t + T, t, y)$$

is a near identity map for all $t \in [t_0, t_0 + NT]$ and $y \in U$ in the sense that there exists a small positive constant ε such that $f(t, y) := (\varphi_T(t, y) - y)/\varepsilon$ and its derivatives up to a certain order Q are of moderate size.

Proceeding similarly to the standard extension of RK methods from autonomous to non-autonomous differential equations, we can consider the natural extension of MRRK methods to the non-autonomous map $\widehat{\varphi}_T : [t_0, t_0+NT]\times U \to \mathbb{R} \times \mathbb{R}^m$

$$\widehat{\varphi}_T : (t, y) \mapsto (t + T, \varphi_T(t, y)) = (t + T, y(t + T, t, y)).$$

The equations of an s-stage MRRK method with coefficients (A, b) that approximate $\widehat{\varphi}_T^N$ can be written as follows

$$T_i = t_0 + c_i NT, \quad \text{for } i = 1, \ldots, s, \tag{29a}$$

$$Y_i = y_0 + N \sum_{j=1}^{s} a_{ij}(\varphi_T(T_j, Y_j) - Y_j), \quad \text{for } i = 1, \ldots, s, \tag{29b}$$

$$t_N = t_0 + NT, \tag{29c}$$

$$y_N = y_0 + N \sum_{i=1}^{s} b_i(\varphi_T(T_i, Y_i) - Y_i), \tag{29d}$$

where $c_i := \sum_{j=1}^{s} a_{ij}$ for $i = 1, \ldots, s$.

Assuming that the MRRK method (29) has order $p > 1$ for autonomous near identity maps $\varphi_T(y)$, the error in the approximation y_N given by (29) to $\varphi_T^N(t_0, y_0)$ does not behave in general as $\mathcal{O}\left((\varepsilon N)^{p+1}\right)$. Consider, e.g., the simple non-autonomous differential equation

$$\frac{dy}{dt} = \sin(t) - \varepsilon e^{-t}, \qquad y(t_0) = y_0.$$

Taking $T = 2\pi$ we have

$$\varphi_{2\pi}(t_0, y_0) = y_0 + \varepsilon e^{-t_0}\left(e^{-2\pi} - 1\right), \tag{30}$$

and

$$\varphi_{2\pi}^{N}(t_0, y_0) = y_0 + \varepsilon e^{-t_0}\left(e^{-N2\pi} - 1\right). \tag{31}$$

The equations of the second order Gauss MRRK method ($s = 1$), see Table 1, applied to (30) provide the approximation to (31) given by

$$y_N = y_0 + N\varepsilon e^{-(t_0+N2\pi c_1)}\left(e^{-2\pi} - 1\right) \tag{32}$$

where $c_1 = 1/2 - 1/(2N)$. It follows from (31) and (32) that

$$\varphi_{2\pi}^{N}(t_0, y_0) - y_N = 2\varepsilon N e^{-t_0-N\pi}\left(\sinh(\pi) - \frac{\sinh(N\pi)}{N}\right).$$

Therefore, the second order Gauss MRRK method ($s = 1$) behaves as a first order method in $h = \varepsilon N$ for the non-autonomous near identity map (30).

To explain the failure of the order of algorithm (29) for non-autonomous near identity maps, observe that the first component of $\widehat{\varphi}_T$ behaves as a near identity map only when T is sufficiently small. In particular, for the above example $|\varphi_T(t_0, y_0) - y_0| = \mathcal{O}(\varepsilon)$ whereas $T = 2\pi$. Clearly if $T = \mathcal{O}(\varepsilon)$, then $\widehat{\varphi}_T$ would be a near identity map and then the theory of order would hold.

In view of this previous example one is tempted to overcome this difficulty by scaling the independent variable $t = s/\varepsilon$ so that $S := \varepsilon T = \mathcal{O}(\varepsilon)$. However, as we will see next, such a scaling does not ensure the near identity behavior of the extended transformed map $\widehat{\Psi}_S(s, y) := \widehat{\varphi}_{S/\varepsilon}(s/\varepsilon, y)$ and the required boundedness of all derivatives of $(\Psi_S(s, y) - y)/\varepsilon$ up to a certain order. Consider, e.g., the second-order differential equation

$$y''(t) - y(t) = 2\varepsilon\cos(t) - 2\varepsilon t\sin(t), \quad y(t_0) = y_0,\ y'(t_0) = y_0', \tag{33}$$

where ε is a small constant parameter. The map $\varphi_T(t, y, y')$ associated to $(y(t), y'(t)) \to (y(t+T), y'(t+T))$ for $T = 2\pi$, where $y(t) = y(t, t_0, y_0, y_0')$ is the general solution of (33), is given by the non-autonomous near identity map

$$\varphi_{2\pi}(t_0, y_0, y_0') = \left(y_0 + 2\pi\varepsilon\sin(t_0),\, y_0' + 2\pi\varepsilon\cos(t_0)\right).$$

By introducing the new independent variable $s = \varepsilon t$ we have $\dot{y}_0 = \varepsilon^{-1} y_0'$, $s_0 = \varepsilon t_0$, and the corresponding map $\Psi_S(s, y, y')$ with $S = \varepsilon T = 2\pi\varepsilon$ is

$$\Psi_{2\pi\varepsilon}(s_0, y_0, \dot{y}_0) = (y_0 + 2\pi\varepsilon\sin(s_0/\varepsilon),\, \dot{y}_0 + 2\pi\cos(s_0/\varepsilon)).$$

Clearly the map $\Psi_{2\pi\varepsilon}$ is not a near identity map. Furthermore, its derivatives with respect to s_0 are not of moderate size.

The above considerations show that the extension (29) of MRRK methods (4) to non-autonomous maps does not retain in general its order properties.

A special situation is when the function $g(t, y)$ of (28) is periodic with respect to t with period T. In this case if $y(t)$ is a solution of (28), $y(t+T)$ is also a solution and therefore $y(t+T, t_0+T, y_0) = y(t, t_0, y_0)$ for all (t_0, y_0). This implies that

$$\varphi_T(t_0 + T, y_0) = y(t_0 + 2T, t_0 + T, y_0) = y(t_0 + T, t_0, y_0) = \varphi_T(t_0, y_0),$$

i.e., $\varphi_T(t, y)$ is T-periodic with respect to t. We have

$$\varphi_T^2(t_0, y_0) = \varphi_{2T}(t_0, y_0) = \varphi_T(t_0 + T, \varphi_T(t_0, y_0)) = \varphi_T(t_0, \varphi_T(t_0, y_0)),$$

and more generally

$$\varphi_T^N(t_0, y_0) = \varphi_{NT}(t_0, y_0) = \varphi_T(t_0, \varphi_T^{N-1}(t_0, y_0)).$$

Thus t_0 can be considered as a fixed constant. In view of this fact in the application of an MRRK method to the T-periodic map $\varphi_T(t, y)$, we can consider t as a fixed parameter and the approximation y_N to $\varphi_T^N(t_0, y_0)$ given by

$$Y_i = y_0 + N \sum_{j=1}^{s} a_{ij}(\varphi_T(t_0, Y_j) - Y_j), \quad \text{for } i = 1, \ldots, s,$$

$$y_N = y_0 + N \sum_{i=1}^{s} b_i(\varphi_T(t_0, Y_i) - Y_i).$$

Clearly the order of the MRRK method (4) is retained.

7 Numerical experiments with the harmonic oscillator

To illustrate some aspects of the theory of MRRK methods developed in the above sections we first consider the linear system of differential equations for the harmonic oscillator

$$y' = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} y. \tag{34}$$

All solutions of (34) are 2π-periodic and therefore the 2π-flow map $\varphi_{2\pi}(y)$ is simply the identity map $\varphi_{2\pi}(y) = y$. However, if we integrate (34) with the Verlet algorithm along a 2π-period with constant step size $\Delta t = 2\pi/n$ (n being a fixed positive integer), the resulting map $\widetilde{\varphi}_{2\pi}(y)$, called the Verlet 2π-flow map hereafter, which is given by

$$\widetilde{\varphi}_{2\pi}(y) = \begin{pmatrix} 1 - \frac{\Delta t^2}{2} & \Delta t \\ -\Delta t \left(1 - \frac{\Delta t^2}{4}\right) & 1 - \frac{\Delta t^2}{2} \end{pmatrix}^n y =: \widetilde{\Gamma}^n y, \tag{35}$$

is a near identity map for small stepsizes $\Delta t = 2\pi/n$, because the Verlet algorithm is a second order method and $\widetilde{\varphi}_{2\pi}(y) - y = \mathcal{O}(\Delta t^2)$.

First we consider the approximation of $\widetilde{\varphi}_{2\pi}^N$ by means of the second order Gauss MRRK method ($s = 1$), see Table 1. Putting $c_1 := 1/2 - 1/(2N)$ the MRRK equations (4) of this method can be written in the form

$$y_N = y_0 + N\left(\varphi_T(c_1 y_N + (1-c_1)y_0) - (c_1 y_N + (1-c_1)y_0)\right). \tag{36}$$

The approximation y_N to $\varphi_T^N(y_0)$ is defined by an implicit equation whose solution has a computational cost which is generally unknown in advance. In particular, if a fixed point iteration is applied to solve (36) with $\varphi_T := \widetilde{\varphi}_{2\pi}$, each iteration requires one Verlet 2π-flow map $\widetilde{\varphi}_{2\pi}$, i.e., n steps of the Verlet algorithm. For $\widetilde{\varphi}_{2\pi}$ given by (35), equation (36) can be solved explicitly leading to

$$y_N = \left((1-c_1)I - c_1\Gamma^n\right)^{-1}\left(-c_1 I + (1-c_1)\Gamma^n\right) y_0 =: \Gamma_N y_0, \tag{37}$$

and its error is

$$\widetilde{\varphi}_{2\pi}^N(y_0) - y_N = (\widetilde{\Gamma}^{nN} - \Gamma_N)y_0.$$

In the same way, the global error after K steps of the second order Gauss MRRK method ($s = 1$) is

$$\widetilde{\varphi}_{2\pi}^{NK}(y_0) - y_{NK} = (\widetilde{\Gamma}^{nNK} - \Gamma_N^K)y_0.$$

In order to give an estimation of these errors independently of the starting value y_0 we introduce the notations

$$\theta := \arctan\left(\frac{\Delta t\sqrt{1-\Delta t^2/4}}{1-\Delta t^2/2}\right) \quad \text{for } n = 2\pi/\Delta t \geq 5,$$

$$P := \begin{pmatrix} \frac{-i}{\sqrt{1-\Delta t^2/4}} & \frac{i}{\sqrt{1-\Delta t^2/4}} \\ 1 & 1 \end{pmatrix}.$$

The matrix $\widetilde{\Gamma}$ of (35) can be written as $\widetilde{\Gamma} = P\Lambda P^{-1}$ with

$$\Lambda := \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix},$$

and therefore $\widetilde{\Gamma}^n = P\Lambda^n P^{-1}$. For the matrix Γ_N of the multi-revolution method (37) we have

$$\Gamma_N = P\begin{pmatrix} \bar{w} & 0 \\ 0 & w \end{pmatrix} P^{-1},$$

with $w := (1-c_1)e^{in\theta}/((1-c_1)-c_1e^{in\theta})$. Hence, for the local error we have

$$\widetilde{\Gamma}^{nN} - \Gamma_N = P \begin{pmatrix} e^{-in\theta N} - \bar{w} & 0 \\ 0 & e^{in\theta N} - w \end{pmatrix} P^{-1}. \tag{38}$$

In view of (38) a measure of the local error is $|e^{in\theta N} - w|$. To give an expansion of this error observe that taking into account $n\Delta t = T = 2\pi$, after some calculations we arrive at the following expansions in powers of $\Delta t^2 N$

$$\begin{aligned} e^{in\theta N} &= 1 + \frac{i\pi}{12}\Delta t^2 N + \frac{\left(27\pi N^{-1} i - 10\pi^2\right)}{2880}(\Delta t^2 N)^2 \\ &\quad + \frac{\left((2025N^{-2}\pi - 140\pi^3)i - 1134N^{-1}\pi^2\right)}{1451520}(\Delta t^2 N)^3 \\ &\quad + \mathcal{O}\left((\Delta t^2 N)^4\right), \\ w &= 1 + \frac{i\pi}{12}\Delta t^2 N + \frac{\left(27\pi N^{-1} i - 10\pi^2\right)}{2880}(\Delta t^2 N)^2 \\ &\quad + \frac{\left((2025N^{-2}\pi + 70N^{-2}\pi^3 - 210\pi^3)i - 1134N^{-1}\pi^2\right)}{1451520}(\Delta t^2 N)^3 \\ &\quad + \mathcal{O}\left((\Delta t^2 N)^4\right). \end{aligned}$$

Therefore,

$$|e^{in\theta N} - w| = \frac{\pi^3}{20736}\left(1 - \frac{1}{N}\right)(\Delta t^2 N)^3 + \mathcal{O}((\Delta t^2 N)^4),$$

and from this expression it is clear that the local error of the 1-stage Gauss MRRK method behaves as $\mathcal{O}((\Delta t^2 N)^3)$ which agrees with the second order of the method. Observe that the Verlet algorithm is symplectic and $\widetilde{\varphi}_{2\pi}(y) = \widetilde{\Gamma}^n y$ is also a linear symplectic map. Furthermore, since Gauss MRRK methods are symplectic, Γ_N is a symplectic matrix that approximates $\widetilde{\Gamma}^{nN}$. The MRRK method (37) does not have any dissipation error and its dispersion error is given by

$$\arg(e^{inN\theta}) - \arg(w) = \frac{\pi^3}{20736}\left(\frac{1}{N} - 1\right)(\Delta t^2 N)^3 + \mathcal{O}((\Delta t^2 N)^4).$$

Its dispersion order is therefore equal to 2.

Similarly the global error after K steps of the MRRK method can be measured by $|e^{in\theta NK} - w^K|$ which can be expanded as

$$|e^{in\theta NK} - w^K| = \frac{\pi^3}{20736}\left(1 - \frac{1}{N}\right)K(\Delta t^2 N)^3 + \mathcal{O}(K^2(\Delta t^2 N)^4).$$

Taking as initial values $y_1(0) = 0.7$, $y_2(0) = 0.8$, $n = 500$, $N = 100$ and $K = 159$, corresponding to a long time interval of length $2\pi NK \approx 10^5$, then

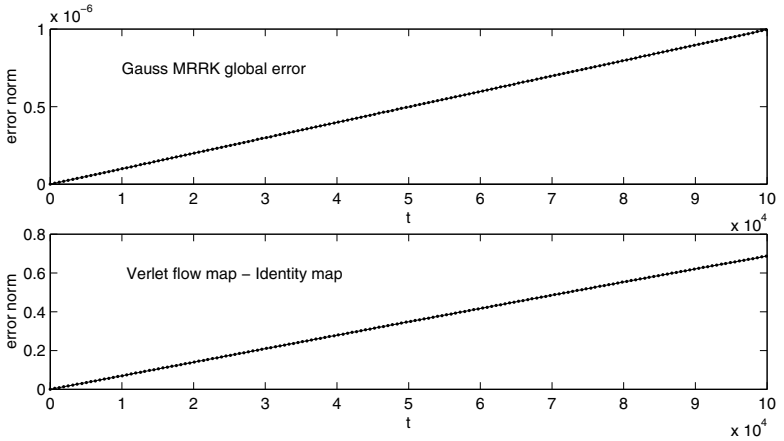

Fig. 1. Errors for 1-stage Gauss MRRK with respect to the Verlet 2π-flow map for the harmonic oscillator

$h := \varepsilon N = \Delta t^2 N = (2\pi)^2/2500 \approx 0.016$ is sufficiently small so that the asymptotic expansions in (7)–(8) are expected to be good approximations. In Fig. 1 we have plotted the global errors $\widetilde{\varphi}_{2\pi}^{Nr} - y_{Nr}$, for $r = 1, \ldots, K$, of the 1-stage Gauss MRRK method for this problem. As can be seen, the global error $\widetilde{\varphi}_{2\pi}^{NK} - y_{NK}$ is of the order of 10^{-6} on the considered time interval. This is negligible compared to the error of Verlet 2π-flow map with respect to the exact 2π-flow map of the harmonic oscillator (the identity map) which is of the order of 1, as can be seen in Fig. 1.

Next we consider the 2-stage explicit Runge's MRRK method defined by the Butcher-tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} - \frac{1}{2N} & \frac{1}{2} - \frac{1}{2N} & 0 \\ \hline & 0 & 1 \end{array}$$

It is a second order MRRK method and in the limit $N \to \infty$ we obtain Runge's RK method of order 2 for ODEs. If we use this method to approximate $\widetilde{\varphi}_{2\pi}^{N}(y_0)$ we obtain

$$y_N = \left(c_1 N^2 \widetilde{\Gamma}^{2n} + (N - 2c_1 N^2)\widetilde{\Gamma}^n + (1 + c_1 N^2 - N)\right) y_0$$

where $c_1 := 1/2 - 1/(2N)$. Proceeding as for the previous method, we have $y_N = P\mathrm{diag}(\bar{v}, v)P^{-1} y_0$ with $v := c_1 N^2 e^{2in\theta} + (n - 2c_1 N^2)e^{in\theta} + (1 + c_1 N^2 - N)$, and the leading term of the local error $|e^{in\theta N} - v|$ behaves as

$$\frac{\pi^3 \Delta t^6 N(N-1)(N-2)}{10368} + \mathcal{O}((\Delta t^2 N)^4),$$

which shows a second order MRRK method in $\Delta t^2 N$. Moreover, after some calculations we obtain

$$|v|^2 = 1 + N(N-1)^2(N-2)\,(1-\cos(n\theta))^2 > 1.$$

This implies that Runge's MRRK method is a non-symplectic method, the MRRK approximations spiral outwards. Furthermore, since $\cos(n\theta) = 1 - \frac{1}{288}\pi^2\Delta t^4 + \mathcal{O}(\Delta t^6)$,

$$|v| = 1 + \frac{\Delta t^8 N(N-1)^2(N-2)\pi^4}{165888} + \mathcal{O}((N\Delta t^2)^5),$$

Runge's MRRK dissipation order is therefore equal to 4.

In the next example we consider a nonlinear perturbation of the linear harmonic oscillator equations (34). More succinctly we consider the autonomous nonlinear second order differential equation

$$y'' + y = \varepsilon y^3.$$

The 2π-flow map associated to this differential equation $\varphi_{2\pi}(y_0, y_0') = \big(y(2\pi, y_0, y_0'), y'(2\pi, y_0, y_0')\big)$ satisfies

$$\|\varphi_{2\pi}(y_0, y_0') - (y_0, y_0')\| = \mathcal{O}(\varepsilon),$$

thus is a near identity map for ε small. To test the behavior of the 2-stage Gauss MRRK method, see Table 1, applied to the map $\varphi_{2\pi}$ we have taken $\varepsilon = 10^{-2}$ and the initial conditions $y(0) = 1$, $y'(0) = 0$. In the MRRK method we have approximated $\varphi_{2\pi}$ by integrating numerically the differential equation with the 2-stage Gauss RK method for ODEs with $n = 150$ steps of length $\Delta t = 2\pi/n$. In Table 9 we give the global error $\|\varphi_{2\pi}^{NK} - y_{NK}\|$ obtained by taking K steps of the MRRK method, each of them advancing N revolutions, in such a way that $NK = 64$. The global error has been obtained approximating the exact solution by means of the expressions

$$\begin{aligned}
\nu &= 1 - \left(\frac{3}{8}\varepsilon + \frac{21}{256}\varepsilon^2 + \frac{81}{2048}\varepsilon^3 + \frac{6549}{262144}\varepsilon^4\right),\\
\eta &= \cos(\nu t),\\
y(t) &= \eta + \eta\left(\frac{1}{8}\varepsilon + \frac{25}{256}\varepsilon^2 + \frac{161}{2048}\varepsilon^3\right) - \eta^3\left(\frac{1}{8}\varepsilon + \frac{29}{256}\varepsilon^2 + \frac{212}{2048}\varepsilon^3\right)\\
&\quad + \eta^5\left(\frac{4}{256}\varepsilon^2 + \frac{55}{2048}\varepsilon^3\right) - \eta^7\frac{1}{512}\varepsilon^3.
\end{aligned}$$

The quotients of global error are successively equal to 13.78, 18.86, 15.63 (close to $2^4 = 16$) and this illustrates that the 2-stage Gauss MRRK method has order 4.

Table 9. MRRK global error

N	K	global error
4	16	$9.51 \cdot 10^{-7}$
8	8	$1.31 \cdot 10^{-5}$
16	4	$2.47 \cdot 10^{-4}$
32	2	$3.86 \cdot 10^{-3}$

8 Conclusions

In this paper a general theory of Runge-Kutta type algorithms that approximate the N-th power φ^N of a near identity map φ at some point by using the map φ at a few $s \ll N$ selected points is developed. In this framework a theory of order is presented and, by introducing suitable simplifying assumptions, high order methods of Gauss, Radau, and Lobatto type are derived for any number of stages. The above theory can be considered in a sense as a generalization of the standard Butcher theory for ODEs. MRRK methods preserving constant Poisson/symplectic structures and reversibility properties are characterized. On the other hand it provides a theoretical background of the so-called multi-revolution Runge-Kutta methods used in some problems of celestial mechanics and in highly oscillatory problems of other fields.

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