HAMILTONIAN SYSTEMS AND SYMPLECTIC INTEGRATORS

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1. INTRODUCTION

Hamiltonian systems arise in many areas of physics, mechanics and engineering sciences, as well as in pure and applied mathematics. In the last years the interest in integrating these systems numerically has increased strongly. Numerical integrators have to conserve the basic and important properties of Hamiltonian systems, and up to now many symplectic integrators are known. But there are further properties to be studied such as stability and conservation of energy.

When integrating dynamical systems it is important to study the properties of the method in comparison with those of the dynamical systems. The numerical methods represent discrete dynamical systems, and hence first, common properties of continuous and discrete dynamical systems in the linear and nonlinear case have to be analyzed. Then mostly a very difficult task is to translate the desired properties to algebraic conditions for the coefficients of the numerical methods.

When solving Hamiltonian systems the property of symplecticness is basic and symplectic integrators of Runge–Kutta type have been studied in detail in the last years (cf. Sanz–Serna and Calvo [12], Görtz and Scherer [4]). Explicit Runge–Kutta methods do not have this property but there exist symplectic Runge–Kutta type methods, which are explicit. In this field one approach was derived from Runge–Kutta methods and the other from Nyström methods applied to second order systems, and the results are closely related to each other.

Stability properties have been studied for second order systems (cf. Hairer [5], van der Houwen and Sommeijer [6], [7]) but not in detail for Hamiltonian systems (cf. McLachlan [8], Qin and Zhang [10]). Conservation of energy means stability, too. It is known that Runge–Kutta methods with stability matrix $M = 0$ or with symmetric $A$–stability function conserve energy when applied to linear Hamiltonian systems, but for the other Runge–Kutta type methods the situation is more complicated (cf. [12]).

In this paper some new ideas about symplectic stability and the relation to energy conservation for Runge–Kutta type methods are discussed. As a test equation the harmonic oscillator

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is used, which is stable but not asymptotically stable. A symplectic Runge–Kutta type method
holds this stability property at least for sufficiently small stepsize $h$. Especially, Runge–Kutta
methods are emphasized but the results partially hold for other types, too (cf. Götz [3]).

Consider the autonomous Hamiltonian system (cf. Arnold [1])

$$\dot{p} = -\frac{\partial H(p, q)}{\partial q}, \quad \dot{q} = \frac{\partial H(p, q)}{\partial p}$$

with Hamiltonian $H = H(p, q)$ being sufficiently smooth.

A Runge–Kutta method $(c, A, b)$ will be applied to the general system, a partitioned Runge–
Kutta method $(c^{(1)}, A^{(1)}, b^{(1)}; c^{(2)}, A^{(2)}, b^{(2)})$ to the separable system with
$H(p, q) = T(p) + V(q)$, a Runge–Kutta–Nyström method $(c, \hat{A}, b, b)$ to the separable and partially linear system with
$T(p) = \frac{1}{2}p^T K p$ and a Runge–Kutta method with symmetric $A$-stability function to the linear
system with $H(u) = \frac{1}{2}u^T Su$. Hence, if we refer to symplectic Runge–Kutta type methods,
keep in mind the four different cases of Hamiltonian systems. The greatest common measure
is the system with

$$H(p, q) = \frac{1}{2}p^T K p + \frac{1}{2}q^T N q,$$

which in the case $K$ and $N$ positive definite will be reduced to the test equation of the harmonic
oscillator

$$\dot{u} = -\nu J u, \quad \nu > 0, \quad u = \begin{pmatrix} p \\ q \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

(1.1)

with Hamiltonian representing the total energy

$$H(u) = \frac{1}{2} u^T u,$$

(1.2)

which is a conserved quantity, i.e., $H(u(t)) = H(u(0))$ for all $t > 0$. Naturally (1.1) is closely
related to $\ddot{q} = -\omega^2 q$ ([5], [6], [7]).

A Runge–Kutta type method, which is always assumed to be consistent, applied to the test
equation (1.1) with initial value $u(0) = u_0$ yields the discrete system

$$u_{m+1} = G(h \nu) u_m, \quad m = 0, 1, 2, \ldots,$$

(1.3)

where with $x = h \nu$ the matrix

$$G(x) = \begin{pmatrix} g_{11}(x) & g_{12}(x) \\ g_{21}(x) & g_{22}(x) \end{pmatrix}$$

consists of rational functions $g_{ij}(x)$, in case of explicit methods only of polynomials ([3]). In
the limiting case it holds $G(0) = I$.

When the solution $u(t) = (p(t), q(t))^T$ of (1.1) with $u(0) = u_0$ is plotted in the phase $(p, q)$-
plane, the parametric curve describes the circle $H(p, q) = H(u_0)$. The solution $\{ u_m \}_{m \geq 0}$ of
(1.3) should have a similar behaviour in the phase $(p, q)$-plane. But conservation of energy
for the discrete system, which means

$$H(u_m) = H(u_0), \quad m = 1, 2, \ldots \quad \text{for all initial values } u(0) = u_0,$$

(1.4)

cannot always be expected.
For Runge–Kutta methods it is $G(x) = R(-xJ)$, where $R(z)$ is the $A$–stability function, and especially, the matrix $G(x)$ has the simple configuration

$$g_{11}(x) = g_{22}(x) = 1 - x^2 b^T (I + x^2 A^2)^{-1} c,$$

$$g_{21}(x) = -g_{12}(x) = x b^T (I + x^2 A^2)^{-1} e,$$

where $e = (1, \ldots, 1)^T$, and the determinant and trace of $G(x)$ satisfy

$$\det G(x) = 1 + ((b^T e)^2 - 2 b^T c) x^2 + O(x^4) \text{ for } x \to 0$$

and

$$\text{tr } G(x) = 2 - 2 b^T c x^2 + O(x^4) \text{ for } x \to 0,$$

respectively.

The transformation (1.3) is symplectic if and only if

$$\det G(x) = 1 \text{ for all permissible } x$$

(poles of $g_{ij}(x)$ have to be taken in consideration), which immediately follows from condition $G^T J G = J$. Hence, symplectic Runge–Kutta type methods satisfy (1.9). Without property (1.9) there exist at most a finite number of $x$ such that $\det G(x) = 1$, i.e., symplecticness does not hold for $x = h \nu \to 0$. For a consistent and symplectic Runge–Kutta method the relation (1.7) implies $2 b^T c = 1$, i.e., the quadrature formula $(c, b)$ has at least order two.

### 2. STABILITY

The test equation (1.1) having the eigenvalues $\mu_{1/2} = \pm i \nu$ is stable but not asymptotically stable for all $\nu$. A linear Hamiltonian system never can be asymptotically stable in the origin. The discrete system (1.3) must have the same property as the test equation. It is stable but not asymptotically stable if and only if the eigenvalues $\lambda_{1/2}(x)$ of $G(x)$ satisfy

$$|\lambda_{1/2}(x)| = 1, \text{ and } \lambda_1(x) = \lambda_2(x) = \pm 1 \text{ implies } G(x) = \pm I.$$  

This request is studied under the assumption that the method is symplectic, which means that at least (1.9) is satisfied. The eigenvalues $\lambda_{1/2}(x)$ are expressed by trace of $G(x)$.

**Lemma 2.1.** For a symplectic Runge–Kutta type method the discrete system (1.3) with $x = h \nu$ is stable but not asymptotically stable if and only if

$$|\text{tr } G(x)| \leq 2, \text{ and } |\text{tr } G(x)| = 2 \text{ implies } G(x) = \pm I.$$  

**Proof.** With (1.9) the eigenvalues of $G(x)$ are given by

$$\lambda_{1/2}(x) = \frac{1}{2} \text{tr } G(x) \pm i \sqrt{1 - \frac{1}{4}(\text{tr } G(x))^2}.$$  

Hence, condition $|\text{tr } G(x)| < 2$ implies

$$|\lambda_1(x)| = |\lambda_2(x)| = 1, \quad \lambda_1(x) \neq \lambda_2(x),$$

and $|\text{tr } G(x)| = 2$ implies $\lambda_1(x) = \lambda_2(x) = \pm 1$. The reversal is given in a similar manner.

The matrix $G$ depends on $x = h\nu$, where $\nu$ is given in (1.1) and the stepsize $h$ of the method has to be chosen. We are interested in determining the size of $h$, where stability is given.

**Theorem 2.2.** For a symplectic Runge-Kutta type method the discrete system (1.3) satisfies

$$|\text{tr } G(x)| < 2 \quad \text{for all sufficiently small } x = h\nu > 0. \quad (2.3)$$

**Proof.** From (1.8) the desired statement follows, since a consistent and symplectic Runge-Kutta method satisfies $2b^Tc = 1$. For partitioned Runge-Kutta methods and Runge-Kutta-Nyström methods the proof is given in a similar way ([3]). \(\Box\)

**Definition 2.3.** For a symplectic Runge-Kutta type method

$$\Gamma = \{x \geq 0 : |\text{tr } G(x)| \leq 2, \text{ and } |\text{tr } G(x)| = 2 \implies G(x) = \pm I\} \quad (2.4)$$

is called the region of symplectic stability.

Treating the test equation (1.1) then the stepsize $h$ of the method has to be chosen such that $x = h\nu \in \Gamma$. The region of symplectic stability $\Gamma$ may be a finite or infinite intervall or a junction of intervalls. Since $\text{tr } G(x)$ is a polynomial, an explicit Runge-Kutta type method never has an infinite region $\Gamma$.

**Corollary 2.4.** For a symplectic Runge-Kutta method there always holds $\Gamma = [0, \infty)$ and conservation of energy (1.4) is satisfied.

**Proof.** Notice the simple configuration of $G(x)$ (see (1.5) and (1.6)) then it follows

$$\lambda_{1/2}(x) = g_{11}(x) \pm i|g_{21}(x)|, \quad |\lambda_{1/2}(x)|^2 = g_{11}^2(x) + g_{21}^2(x) = \det G(x) = 1,$$

and hence,

$$|\text{tr } G(x)| \leq |\lambda_1(x)| + |\lambda_2(x)| = 2$$

for all $x > 0$; further $\lambda_1(x) = \lambda_2(x) = \pm 1$ implies $G(x) = \pm I$. Since

$$G^T(x)G(x) = \det G(x)I = I$$

it follows

$$H(u_{m+1}) = \frac{\nu}{2}(G(x)u_m)^T G(x)u_m = H(u_m),$$

which means conservation of energy.
This result cannot be completely extended to partitioned Runge–Kutta and Runge–Kutta–
Nyström methods, namely there is no conservation of energy. Examples show that the discrete
solution \( \{ u_m = (p_m, q_m)^T \}_{m \geq 0} \) plotted in the phase \((p, q)\)-plane corresponds to an ellipse if
and only if \( \hbar \nu \in \Gamma \), in the other case \( \{ ||u_m|| \}_{m \geq 0} \) grows up very rapidly.

**EXAMPLES:**

i) The Gauss–Runge–Kutta methods satisfy \( M = 0 \) (cf. Butcher [2]) and conserve energy
when applied to linear Hamiltonian systems, hence, according to Corollary 2.4 the stability
region is given by \( \Gamma = [0, \infty) \). Consider the one and two stage methods with

\[
\text{tr } G(x) = 2 \frac{1 - \frac{1}{4}x^2}{1 + \frac{1}{4}x^2} \quad \text{and} \quad \text{tr } G(x) = 2 \frac{1 - \frac{5}{12}x^2 + \frac{1}{144}x^4}{1 + \frac{1}{12}x^2 + \frac{1}{144}x^4},
\]

respectively, where \( \text{tr } G(2\sqrt{3}) = -2 \) and \( G(2\sqrt{3}) = -I \) for the two stage method.

ii) The trapezoidal rule having a symmetric \( A \)-stability function possesses the same region
\( \Gamma = [0, \infty) \) as the one stage Gauss method.

iii) The explicit partitioned Runge–Kutta method \((1|1|1||0|0|1)\) (Ruth [11]) yields the
matrix \( G(x) \) with

\[
g_{11}(x) = 1, \quad g_{22}(x) = 1 - x^2, \quad g_{21}(x) = -g_{12}(x) = x,
\]

and \( \det G(x) = 1 \), \( \text{tr } G(x) = 2 - x^2 \), \( G(2) \neq \pm I \), and hence, \( \Gamma = [0, 2) \).

For example, if \( x = 1 \) then the points \( u_m = G^m(1)u_0, \ m = 0, 1, 2, \ldots, \) lie on an ellipse
with twisted axes, e.g.,

\[
u_0 = (1, 0)^T, \ v_1 = (1, 1)^T, \ v_2 = (0, 1)^T, \ v_3 = (-1, 0)^T, \ v_4 = (-1, -1)^T, \ v_5 = (0, -1)^T, \ v_6 = u_0
\]

lie on \( p^2 - pq + q^2 = 1 \).

iv) The explicit partitioned Runge–Kutta method (McLachlan and Atela [9])

\[
\begin{pmatrix}
1 - \alpha & 1 - \alpha & 0 & 1 - \alpha & 0 & 0 & \alpha \\
\alpha & 1 - \alpha & \alpha & \alpha & 0 & 0 & 1 - \alpha
\end{pmatrix}, \quad \alpha = \frac{1}{2}\sqrt{2}
\]

yields the matrix \( G(x) \) with

\[
g_{11}(x) = 1 - \frac{1}{2}x^2, \ g_{22}(x) = g_{11}(x) + \frac{1}{4}(3 - 4\alpha)x^4, \ g_{21}(x) = -g_{12}(x) = x - \frac{1}{2}(1 - \alpha)x^3,
\]

and hence, \( \det G(x) = 1 \) and \( \text{tr } G(x) = 2 - x^2 + \frac{1}{4}(3 - 4\alpha)x^4 \). With the abbreviations

\[
\beta = 3 - 4\alpha, \ \delta = \sqrt{-4\beta + 1}, \ \rho_1 = \frac{2(1-\delta)}{\beta}, \ \rho_2 = \frac{2(1+\delta)}{\beta} \quad \text{and} \quad \rho_3 = \frac{4}{\beta}
\]

the stability region is given by

\[
\Gamma = [0, \sqrt{\rho_1}) \cup (\sqrt{\rho_2}, \sqrt{\rho_3}) = [0, 2.26\ldots) \cup (4.26\ldots, 4.82\ldots).
\]
3. OUTVIEW

The behaviour of the discrete solutions obtained by partitioned Runge–Kutta and Runge–Kutta–Nyström methods with $h\nu \in \Gamma$ should be studied in detail in context with backward error analysis. The elliptical form of the approximate solution in the phase $(p, q)$–plane indicates that the discrete system conserves energy of a perturbed Hamiltonian problem. Furthermore, the stability investigations should be extended to nonlinear Hamiltonian systems with equilibrium points, for example with Hamiltonian $H(p, q) = \sum \nu_i (p_i^2 + q_i^2) + \tilde{V}(q)$, where $\tilde{V}(q)$ contains higher order terms of the $q_i$, such as the Hénon–Heiles problem or a simple type of the Duffing equation. These topics are investigated in a forthcoming paper.

REFERENCES