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QUADRATIC INVARIANTS AND SYMPLECTIC STRUCTURE OF GENERAL LINEAR METHODS[*1)]

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Abstract

In this paper, we present some invariants and conservation laws of general linear methods applied to differential equation systems. We show that the quadratic invariants and symplecticity of the systems can be extended to general linear methods by a tensor product, and show that general linear methods with the matrix M=0 inherit in an extended sense the quadratic invariants possessed by the differential equation systems being integrated and preserve in an extended sense the symplectic structure of the phase space in the integration of Hamiltonian systems. These unify and extend existing relevant results on Runge-Kutta methods, linear multistep methods and one-leg methods. Finally, as special cases of general linear methods, we examine multistep Runge-Kutta methods, one-leg methods and linear two-step methods in detail.

Key words: Quadratic invariants, Symplecticity, General linear methods, Hamiltonian systems.

1. Introduction

Investigating whether a numerical method inherits some dynamical properties possessed by the differential equation systems being integrated is an important field of numerical analysis and has received much attention in recent years [1-10,13,16-24,26,27]. See the review articles of Sanz-Serna[9] and Section II.16 of Hairer et. al.[2] for more detail concerning the symplectic methods. Most of the work on canonical integrators has dealt with one-step formulae such as Runge-Kutta methods(RKMs)[2,3,6,7-10,13,18,20-22,24,26] and Runge-Kutta-Nyström methods (RKNMs)[1,2,9,17]. The study of canonical multistep methods has been restricted to linear multistep methods(LMMs) and one-leg methods(OLMs)[2,4,5,16,18,23,27]. Moreover, Cooper[7] has shown that Runge-Kutta methods with algebraic stability matrix M=0 preserve the quadratic invariants of the systems, and Sanz-Serna[10] and Lasagni[6] have shown them to be symplectic when applied to Hamiltonian systems. Eirola and Sanz-Serna[23] have shown that, for symmetric one-leg methods, the quadratic invariants and symplecticity of the systems can be extended to one-leg methods by a tensor product. Eirola[24] demonstrated that all these results follow from a general monotonicity property of these methods for quadratic forms. Bochev and Scovel[18] showed that symplecticity follows from the fact that these methods preserve quadratic integral invariants and are closed under differentiation and restriction to closed subsystems, furthermore pointed out that though general linear methods are closed under both differentiation and restriction to closed subsystems, it is difficult to determine the form of the quadratic invariants to be preserved by general linear methods simultaneously with the conditions on the coefficients of the methods which will guarantee the preservation of these invariants.

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The main purpose of the present paper is to answer the questions from Bochev and Scovel[18] and to unify and extend the existing results in [6,7,10,23] and to investigate under which conditions a general linear method(GLM) is symplectic in an extended sense when applied to Hamiltonian systems of differential equations and under what conditions a GLM inherits the quadratic invariants possessed by the differential equation systems being integrated.

Consider the following system of differential equations on R^{2N}[25]

$$\begin{cases} \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} = f_i(p,q), & i = 1,2,\ldots,N, \\ \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} = g_i(p,q), & i = 1,2,\ldots,N, \end{cases} \tag{1.1}$$

where $H(p,q)$ with

$$p = (p_1, p_2, \cdots, p_N)^T, \quad q = (q_1, q_2, \cdots, q_N)^T$$

is some real valued smooth function on R^{2N}. We call (1.1) a canonical system of differential equations with Hamiltonian H. We can write (1.1) in the vector form

$$\begin{cases} \frac{dp}{dt} = f(p,q), \\ \frac{dq}{dt} = g(p,q), \end{cases} \tag{1.1$'$}$$

where

$$f(p,q) = (f_1(p,q), f_2(p,q), \ldots, f_N(p,q))^T, \quad g(p,q) = (g_1(p,q), g_2(p,q), \ldots, g_N(p,q))^T.$$

Let $p_i = x_i, q_i = x_{i+N}, i = 1,2,\ldots,N$,

$$x = (x_1, x_2, \cdots, x_{2N})^T, \quad \frac{\partial H}{\partial x} = (\frac{\partial H}{\partial x_1}, \frac{\partial H}{\partial x_2}, \ldots, \frac{\partial H}{\partial x_{2N}})^T \in R^{2N}.$$

Then (1.1) follows that

$$\frac{dx}{dt} = J\frac{\partial H}{\partial x} \tag{1.2}$$

with

$$J = [J_{ij}] = \begin{pmatrix} 0 & -I_N \\ I_N & 0 \end{pmatrix}, \tag{1.3}$$

here and in the following text, I_l denotes the $l \times l$ identity matrix, $l = 1,2,\cdots$. The phase space R^{2N} is equipped with a standard symplectic structure defined by the fundamental differential 2-form[21]

$$\omega = \frac{1}{2} J dx \wedge dx = dp \wedge dq = \sum_{i=1}^{N} dp_i \wedge dq_i,$$

where the symbol $\wedge$ denotes exterior product. Let ψ be a diffeomorphism of R^{2N},

$$x = (p^T, q^T)^T \rightarrow \psi(x) = (\psi_1(x), \psi_2(x), \ldots, \psi_{2N}(x))^T = (\hat{p}^T(p,q), \hat{q}^T(p,q))^T.$$

ψ is called a symplectic transformation if ψ preserves the 2-form ω, i.e.,

$$\sum_{i=1}^{N} d\hat{p}_i \wedge d\hat{q}_i = \sum_{i=1}^{N} dp_i \wedge dq_i. \tag{1.4}$$

This is equivalent to the condition that

$$(\frac{\partial \psi}{\partial x})^T J (\frac{\partial \psi}{\partial x}) \equiv J, \tag{1.5}$$

i.e. the Jacobian matrix $\frac{\partial\psi}{\partial x}$ is symplectic, where

$$\frac{\partial\psi}{\partial x} = \begin{pmatrix} \frac{\partial\hat{p}}{\partial p} & \frac{\partial\hat{p}}{\partial q} \\ \frac{\partial\hat{q}}{\partial p} & \frac{\partial\hat{q}}{\partial q} \end{pmatrix}.$$

We now consider the real system of differential equations of the general form

$$\frac{dy}{dt} = \tilde{f}(y), \tag{1.6}$$

where $y \in R^m$, $\tilde{f} : R^m \to R^m$ is sufficiently smooth, and y(t) is assumed to be a true solution of (1.6). For solving (1.6), consider the r-value s-stage general linear method[2,12,14,15]

$$\begin{cases} Y_i^{(n)} = h\sum\limits_{j=1}^{s} c_{ij}^{11}\tilde{f}(Y_j^{(n)}) + \sum\limits_{j=1}^{r} c_{ij}^{12} y_j^{(n-1)}, \qquad i = 1,2,\ldots,s, \\ y_i^{(n)} = h\sum\limits_{j=1}^{s} c_{ij}^{21}\tilde{f}(Y_j^{(n)}) + \sum\limits_{j=1}^{r} c_{ij}^{22} y_j^{(n-1)}, \qquad i = 1,2,\ldots,r, \end{cases} \tag{1.7}$$

where $h\rangle 0$ is the given stepsize, c_{ij}^{IJ} are real constants, the vectors $Y_i^{(n)}$ are the internal stages of the current step and are approximations to $y(t_n + \mu_i h)$, the vectors $y_i^{(n)}$ are the external stages which contain all information from the previous step necessary for the computation of the new approximation and are approximations to $H_i(t_n + \nu_i h)$, $t_n = nh$, μ_i and ν_i are real constants, each $H_i(t_n + \nu_i h)$ denotes a piece of information about the true solution $y(t)$. Let

$$\begin{cases} y^{(n)} = ({y_1^{(n)}}^T, {y_2^{(n)}}^T, \ldots, {y_r^{(n)}}^T)^T \in R^{mr}, \\ Y^{(n)} = ({Y_1^{(n)}}^T, {Y_2^{(n)}}^T, \ldots, {Y_s^{(n)}}^T)^T \in R^{ms}, \\ F(Y^{(n)}) = h(\tilde{f}(Y_1^{(n)})^T, \tilde{f}(Y_2^{(n)})^T, \ldots, \tilde{f}(Y_s^{(n)})^T)^T \in R^{ms}, \\ C_{IJ} = [c_{ij}^{IJ}], \qquad \tilde{C}_{IJ} = C_{IJ} \otimes I_m, \qquad I, J = 1, 2, \end{cases} \tag{1.8}$$

where the symbol $A \otimes B$ denotes Kronecker product of the matrices A and B. Then the method (1.7) can be written in more compact form

$$\begin{cases} Y^{(n)} = \tilde{C}_{11}F(Y^{(n)}) + \tilde{C}_{12}y^{(n-1)}, \\ y^{(n)} = \tilde{C}_{21}F(Y^{(n)}) + \tilde{C}_{22}y^{(n-1)}. \end{cases} \tag{1.9}$$

2. Quadratic Invariants

In this section we consider the question of whether the method (1.7) inherits in some sense the quadratic invariants possessed by the differential system (1.6) being integrated. At first, we consider a simple special case of linear Hamiltonian systems

$$y' = JSy \tag{2.1}$$

on $R^m, m = 2N$, where S is an $m \times m$ real symmetric positive definite matrix and J an $m \times m$ skew-symmetric matrix defined by (1.3). Then the Hamiltonian of (2.1) is

$$H(y) = \frac{1}{2}y^T Sy$$

and it easily follows that $\frac{d}{dt}H(y) = 0$. This shows conservation of the Hamiltonian, i.e. conservation of the energy of the system. However, for a nonlinear Hamiltonian system, the Hamiltonian is not always a quadratic form. Therefore, conservation of the quadratic forms doesn't mean conservation of the Hamiltonian i.e. energy. Sanz-Serna[10] has pointed out that a Runge-Kutta scheme with the stability matrix M=0 leads to exact conservation of the energy and symplectic structure when applied to linear Hamiltonian systems, but can't lead to conservation of the energy when applied to nonlinear Hamiltonian systems.

Let now φ be a continuous bilinear map from $R^m \times R^m$ to R, and $\phi(y) := \varphi(y,y)$ the corresponding quadratic map. Assume $\phi(y)$ is an invariant quantity of the system (1.6), i.e. for any solution y(t) of (1.6), $\phi(y(t))$ is time-independent. Moreover, this is true iff for all y,

$$\varphi(y, \tilde{f}(y)) + \varphi(\tilde{f}(y), y) = 0. \tag{2.2}$$

If the system (1.6) is numerically integrated with the method (1.7), it is natural to ask whether the quadratic invariant $\phi(y)$ can be extended to the method (1.7)? We can result in the following conclusion.

Theorem 2.1. *Assume that there exists a non-zero real symmetric $r\times r$ matrix $G = [g_{ij}]$ and a real diagonal $s\times s$ matrix $D = diag(d_1, d_2, \ldots, d_s)$ such that the matrix*

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = 0, \tag{2.3}$$

where

$$M_{11} = G - C_{22}^T G C_{22}, \qquad M_{12} = M_{21}^T = C_{12}^T D - C_{22}^T G C_{21},$$
$$M_{22} = C_{11}^T D + D C_{11} - C_{21}^T G C_{21}.$$

Then the method (1.7) applied to the system (1.6) with the quadratic invariant $\phi(y)$ has the quadratic invariant $\phi_G(y^{(n)})$ with respect to the matrix G, i.e. $\phi_G(y^{(n)})$ is independent of the time-level n, where

$$\phi_G(y^{(n)}) = \sum_{i,j=1}^{r} g_{ij} \varphi(y_i^{(n)}, y_j^{(n)}), \qquad n = 0, 1, 2, \cdots. \tag{2.4}$$

Proof. Along the lines of Burrage and Butcher[12].

Take now $\varphi(\xi, \eta) = \xi^T S \eta$, $\xi, \eta \in R^m$, where S is a nonzero symmetric $m\times m$ matrix, then $\phi(y) = y^T S y$. Assume $\phi(y)$ is an invariant quantity of the system (1.6), then

$$y^T S \tilde{f}(y) = 0, \qquad \forall y \in R^m.$$

We can result in the following conclusion from Theorem 2.1:

Corollary 2.1. *Assume the method (1.7) applied to the system (1.6) with the quadratic first integral $\phi(y) = y^T S y$ satisfies the conditions in Theorem 2.1. Then the method has the quadratic invariant $\phi_G(y^{(n)})$ with respect to the matrix G, where*

$$\phi_G(y^{(n)}) = {y^{(n)}}^T (G \otimes S) y^{(n)} = \sum_{i,j=1}^{r} g_{ij} {y_i^{(n)}}^T S y_j^{(n)}.$$

Remark 2.1. Take $\varphi(\xi, \eta) = <\xi, \eta>$, $\xi, \eta \in R^m$, where $< .,. >$ is a standard inner product on R^m. Assume G and D are nonnegative definite. Then M is an algebraically stable matrix given by Burrage and Butcher[12]. Furthermore, assume the system (1.6) satisfies the monotonic condition

$$\varphi(y, \tilde{f}(y)) \leq 0, \qquad \forall y \in R^m.$$

Then from (2.5), we can obtain Theorem 5.1 in [12], i.e. an algebraically stable method (1.7) preserves monotonicity possessed by the system (1.6) and satisfies

$$\phi_G(y^{(n)}) \leq \phi_G(y^{(n-1)}).$$

3. Conservation of Symplectic Structure

Let the method (1.7) be applied to the system (1.1). We consider any given calculating step $(t-h,(u^T,v^T)^T)\to(t,(y^T,z^T)^T)$:

$$\begin{cases} Y_i=\sum\limits_{j=1}^{s}c_{ij}^{11}k_j+\sum\limits_{j=1}^{r}c_{ij}^{12}u_j, & i=1,2,\dots,s,\\ y_i=\sum\limits_{j=1}^{s}c_{ij}^{21}k_j+\sum\limits_{j=1}^{r}c_{ij}^{22}u_j, & i=1,2,\dots,r,\end{cases} \tag{3.1}$$

$$\begin{cases} Z_i=\sum\limits_{j=1}^{s}c_{ij}^{11}l_j+\sum\limits_{j=1}^{r}c_{ij}^{12}v_j, & i=1,2,\dots,s,\\ z_i=\sum\limits_{j=1}^{s}c_{ij}^{21}l_j+\sum\limits_{j=1}^{r}c_{ij}^{22}v_j, & i=1,2,\dots,r,\end{cases} \tag{3.2}$$

where

$$\begin{aligned} k_j&=hf(Y_j,Z_j), & l_j&=hg(Y_j,Z_j), \quad 1\le i\le s,\\ u&=(u_1^T,u_2^T,\dots,u_r^T)^T\in R^{Nr}, & v&=(v_1^T,v_2^T,\dots,v_r^T)^T\in R^{Nr},\\ y&=(y_1^T,y_2^T,\dots,y_r^T)^T\in R^{Nr}, & z&=(z_1^T,z_2^T,\dots,z_r^T)^T\in R^{Nr},\\ y_i&=(y_i^1,y_i^2,\dots,y_i^N)^T\in R^N, & z_i&=(z_i^1,z_i^2,\dots,z_i^N)^T\in R^N,\\ u_i&=(u_i^1,u_i^2,\dots,u_i^N)^T\in R^N, & v_i&=(v_i^1,v_i^2,\dots,v_i^N)^T\in R^N,\end{aligned}$$

y_i and z_i are the numerical solutions of the true solution p(t) and q(t) at a point t respectively when u_i and v_i are the numerical solutions of the true solution p(t-h) and q(t-h) at a point t-h. We define a map $\tilde{\varphi}$ on R^{2Nr}

$$\tilde{\varphi}:\begin{pmatrix} u\\ v\end{pmatrix}\to\begin{pmatrix} y\\ z\end{pmatrix}.$$

It is clear that the map $\tilde{\varphi}$ only depends on the method (1.7).

Definition 3.1. *Assume that there exists a real nonsingular symmetric $r\times r$ matrix $G=[g_{ij}]$ such that the mapping $\tilde{\varphi}$ is a symplectic transformation, i.e., satisfies the equality*

$$\sum_{i,j=1}^{r}g_{ij}dy_i\wedge dz_j=\sum_{i,j=1}^{r}g_{ij}du_i\wedge dv_j, \tag{3.3}$$

where

$$dy_i\wedge dz_j=\sum_{l,m=1}^{N}J_{lm}dy_i^l\wedge dz_j^m, \qquad du_i\wedge dv_j=\sum_{l,m=1}^{N}J_{lm}du_i^l\wedge dv_j^m.$$

Then the method corresponding to the mapping $\tilde{\varphi}$ is said to be symplectic (about the matrix G).

Remark 3.1. It is clear that the differential 2-form

$$\omega_G=\sum_{i,j=1}^{r}g_{ij}dy_i\wedge dz_j$$

is closed and nondegenerate. Thus ω_G is a symplectic structure on R^{2Nr}, and (R^{2Nr},ω_G) is a symplectic manifold [25].

Remark 3.2. It is easy to prove

$$\sum_{i,j=1}^{r}g_{ij}dy_i\wedge dz_j=\frac{1}{2}(G\otimes J)d\bar{a}\wedge d\bar{a}, \tag{3.4a}$$

$$\sum_{i,j=1}^{r} g_{ij} du_i \wedge dv_j = \frac{1}{2}(G\otimes J)da\wedge da, \tag{3.4b}$$

where

$$a = (a_1^T, a_2^T, \ldots, a_r^T)^T, \qquad \bar{a} = (\bar{a}_1^T, \bar{a}_2^T, \ldots, \bar{a}_r^T)^T,$$
$$\bar{a}_i = (y_i^T, z_i^T)^T, \quad a_i = (u_i^T, v_i^T)^T, \qquad i = 1, 2, \ldots, r.$$

Thus the equality (3.3) is equivalent to that

$$(G\otimes J)da\wedge da = (G\otimes J)d\bar{a}\wedge d\bar{a}.$$

This means that the quadratic form $G\otimes J d\bar{a}\wedge d\bar{a}$ is an invariant quantity of the system (1.1).

Furthermore, the mapping $\tilde{\varphi}$ induces, for each 2-form ω_G on R^{2Nr}, a 2-form $\tilde{\varphi}^*\omega_G$ on R^{2Nr}

$$\begin{aligned}\tilde{\varphi}^*\omega_G(a) &= \tfrac{1}{2}(G\otimes J)d\tilde{\varphi}(a)\wedge d\tilde{\varphi}(a)\\ &= \tfrac{1}{2}(G\otimes J)\tilde{\varphi}_a da\wedge \tilde{\varphi}_a da\\ &= \tfrac{1}{2}\tilde{\varphi}_a^T(G\otimes J)\tilde{\varphi}_a da\wedge da.\end{aligned}$$

Because $\omega_G(a) = \frac{1}{2}(G\otimes J)da\wedge da$, the mapping $\tilde{\varphi}$ is a canonical transformation[25] iff

$$\tilde{\varphi}_a^T(G\otimes J)\tilde{\varphi}_a = G\otimes J,$$

i.e. the Jacobian $\tilde{\varphi}_a = \frac{\partial \bar{a}}{\partial a}$ is a $G\otimes J$-symplectic matrix[4,25]. This is equivalent that the mapping $\tilde{\varphi}$ preserves the symplectic structure ω_G , i.e. the formula (3.3) holds.

If G is singular, then ω_G is not a symplectic structure but only a possion structure in the associated extended phase space, at this time, $\tilde{\varphi}$ defines a possion mapping in R^{2Nr} with respect to the structure matrix $G\otimes J$, and when $M = 0$, it will preserves the possion structure ω_G.

Theorem 3.1. *Assume that there exists a real nonsingular symmetric $r\times r$ matrix $G = [g_{ij}]$ and a real diagonal $s\times s$ matrix $D = diag(d_1, d_2, \ldots, d_s)$ such that (2.3) holds. Then the method (1.7) is symplectic (about the matrix G).*

Proof. Along the lines of Burrage and Butcher[12].

Corollary 3.1. *Assume the conditions in Theorem 3.1 are satisfied. Then the mapping $\tilde{\varphi}$ is a canonical transformation.*

Proof. On one hand, Corollary 3.1 can follow from Theorem 3.1 and Remark 3.2; On the other hand, notice that the Jacobian matrix of $\frac{\partial \tilde{f}}{\partial x}$ is infinitesimally symplectic[4,25], i.e. $J\frac{\partial \tilde{f}}{\partial x} + (\frac{\partial \tilde{f}}{\partial x})^T J = 0$, where $x = (p^T, q^T)^T$, $\tilde{f}(p,q) = (f^T(p,q), g^T(p,q))^T$. It is not difficult for us to give a direct proof of Corollary 3.1.

Remark 3.3. In conclusion, for the method (1.7) Theorem 2.1 and 3.1 and Remark 2.1 have showed that there are some internal relationships between the algebraic stability proposed by Burrage and Butcher [11,12] and the quadratic form and symplectic structure by the present paper. Therefore they can be dealt with within the same theoretical framework.

As special examples, in Section 4,5 and 6 we will investigate in detail whether multistep Runge-Kutta methods (MRKMs),OLMs and linear two-step methods satisfy the conditions assumed by Theorem 2.1 and 3.1.

4. Multistep Runge-Kutta Methods

Writing a MRKM[11,14-15] characterized by

$$\begin{cases} Y_i^{(n)} = h\sum\limits_{j=1}^{s} b_{ij}\tilde{f}(Y_j^{(n)}) + \sum\limits_{j=1}^{r} a_{ij}y_{j+n-1}, & i = 1, 2, \ldots, s,\\ y_{n+r} = h\sum\limits_{j=1}^{s} \gamma_j\tilde{f}(Y_j^{(n)}) + \sum\limits_{j=1}^{r} \alpha_j y_{j+n-1}, & i = 1, 2, \ldots, r \end{cases} \tag{4.1}$$

as a general linear method (1.7) we have

$$y_{j+n-1} = y_j^{(n-1)}, \qquad y_{n+r} = y_r^{(n)}, \qquad y(t_n + ih) = H_i(t_n + (i-1)h),$$

$$C_{11} = [b_{ij}] \in R^{s\times s}, \qquad C_{12} = [a_{ij}] \in R^{s\times r},$$

$$C_{21} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \\ \gamma_1 & \gamma_2 & \dots & \gamma_s \end{pmatrix} \in R^{r\times s}, \qquad C_{22} = \begin{pmatrix} 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \\ \alpha_1 & \alpha_2 & \dots & \alpha_r \end{pmatrix} \in R^{r\times r},$$

where $b_{ij}, a_{ij}, \gamma_i, \alpha_i$ are real constants. Let

$$\gamma = (\gamma_1, \gamma_2, \dots, \gamma_s)^T \in R^s, \quad \alpha = (\alpha_1, \alpha_2, \dots, \alpha_r)^T \in R^r.$$

Furthermore, throughout this section we always assume that

$$\sum_{j=1}^{r} \alpha_i = 1, \quad \sum_{j=1}^{r} a_{ij} = 1, \qquad i = 1, 2, \dots, s, \tag{4.2a}$$

$$\mu_i \neq \mu_j \quad \textit{whenever} \quad i \neq j, \tag{4.2b}$$

$$\gamma_i \neq 0, \quad i = 1, 2, \dots, s, \tag{4.2c}$$

where the relation (4.2a) is the preconsistency condition. For the family of MRKMs given by (4.1) one can easily show

$$(M_{11})_{ij} = g_{ij} - g_{rr}\alpha_i\alpha_j - g_{r,j-1}\alpha_i - g_{i-1,r}\alpha_j - g_{i-1,j-1}, \quad i, j = 1, 2, \dots, r, \tag{4.3}$$

$$(M_{21})_{ij} = (M_{12})_{ji} = -g_{rr}\gamma_i\alpha_j - g_{r,j-1}\gamma_i + a_{ij}d_i, \; j = 1, 2, \dots, r, i = 1, 2, \dots, s, \tag{4.4}$$

$$(M_{22})_{ij} = -g_{rr}\gamma_i\gamma_j + d_i b_{ij} + d_j b_{ji}, \quad i, j = 1, 2, \dots, s, \tag{4.5}$$

where $g_{i0} = g_{0i} = 0, i = 0, 1, 2, \dots, r$. Notice that G and γ_i are not equal to 0. It follows from Theorem 5.3 in [12] that $M = 0$ iff

$$\begin{cases} g_{rr} = 2\kappa\lambda, \quad g_{r,j-1} = \kappa(a_j - 2\lambda\alpha_j), \qquad j = 2, 3, \dots, r, \\ g_{ij} = g_{i-1,j-1} + \kappa(a_j\alpha_i + \alpha_j a_i - 2\lambda\alpha_i\alpha_j), \qquad i, j = 1, 2, \dots, r, \\ \kappa = \sum_{j=1}^{r} g_{rj} \neq 0, \end{cases} \tag{4.6}$$

$$d_i = \kappa\gamma_i, \qquad i = 1, 2, \dots, s, \tag{4.7}$$

$$\begin{cases} a_j := a_{kj} = a_{lj}, \quad k \neq l, k, l = 1, 2, \dots, s, \quad j = 1, 2, \dots, r, \\ b_{ii} = \lambda\gamma_i, \qquad i = 1, 2, \dots, s, \\ a_1 = 2\lambda\alpha_1, \quad a_2 = 2\lambda\alpha_2 + \alpha_1 a_r, \\ \gamma_i b_{ij} + \gamma_j b_{ji} - 2\lambda\gamma_i\gamma_j = 0, \qquad i, j = 1, 2, \dots, s, \end{cases} \tag{4.8}$$

where λ is a real constant. Furthermore, it follows from the second formula in (4.6) that

$$\begin{cases} g_{ii} = 2\kappa(\lambda - \sum_{m=i+1}^{r} (\alpha_m a_m - \lambda\alpha_m^2)), \\ g_{r-l,j-l} = \kappa(a_{j+1} - 2\lambda\alpha_{j+1} - \sigma(j, l)), \\ \sigma(j, l) = \sum_{m=0}^{l-1} (\alpha_{r-m} a_{j-m} + \alpha_{j-m} a_{r-m} - 2\lambda\alpha_{r-m}\alpha_{j-m})), \end{cases} \tag{4.9}$$

where $i = 1, 2, \dots, r-1, \; j = 2, 3, \dots, r-1, \; l = 1, 2, \dots, j-1$. From the above and Theorem 2.1 and 3.1 we have the following conclusion.

Theorem 4.1. *The method (4.1) satisfying (4.8) is symplectic for the system (1.1) about the nonsingular matrix G given by (4.6), and has the quadratic invariant (2.4) for the system (1.6) about the matrix G given by (4.6).*

Remark 4.1. Assume that $G \neq 0$ is diagonal. Then it follows from (4.6)-(4.9) that $\alpha_1\alpha_r = 0$ for $r \geq 2$ and

$$\lambda = 1/2,\ a_j = \alpha_j,\ g_{rr} = \kappa,\ \sum_{k=1}^{r} \alpha_k^2 = 1,\ g_{ii} = \kappa \sum_{k=1}^{i} \alpha_k^2,\ i = 1, 2, \cdots, r-1.$$

Furthermore, let $\alpha_1 > 0$, $\alpha_j \geq 0$, $j = 2, 3, \cdots, r$. We have

$$G = \kappa I_r, \quad \alpha = (1, 0, \ldots, 0)^T, \quad D = \kappa diag(\gamma_1, \gamma_2, \ldots, \gamma_s),$$

$$A = e_s\alpha^T, \qquad diag(\gamma)B + B^T diag(\gamma) - \gamma\gamma^T = 0,$$

where $e_s = (1, 1, \ldots, 1)^T \in R^s$. When r=1, the method (4.1) is an s-stage RKM

$$\begin{array}{c|c} \mu & B \\ \hline & \gamma \end{array}$$

it is symplectic (about the matrix G=(1)) if

$$D = diag(\gamma_1, \gamma_2, \ldots, \gamma_s), \quad diag(\gamma)B + B^T diag(\gamma) - \gamma\gamma^T = 0,$$

and preserves the 2-form ω_G.

5. One-Leg Methods

Consider the one-leg method[12]

$$y_n = \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + \ldots + \alpha_r y_{n-r} + hf(\sum_{i=0}^{r} \beta_i y_{n-i}) \tag{5.1}$$

that can be writen equivalently in the form of the method (1.7) with

$$C_{11} = (\beta_0), C_{21} = (\beta, 0, \ldots, 0)^T, C_{12} = (\frac{\beta_0\alpha_1 + \beta_1}{\beta}, \frac{\beta_0\alpha_2 + \beta_2}{\beta}, \ldots, \frac{\beta_0\alpha_r + \beta_r}{\beta}),$$

$$C_{22} = \begin{pmatrix} \alpha_1 & \alpha_2 & \ldots & \alpha_{r-1} & \alpha_r \\ 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 1 & 0 \end{pmatrix}, \quad y_i^{(n)} = \beta y_{n+1-i}, \quad i = 1, 2, \cdots, r,$$

where $\beta = \sum_{i=0}^{r} \beta_i \neq 0$. It is easy to prove that M=0 if and only if

$$\beta_0 = \sum_{l=1}^{r} \alpha_l \beta_l, \qquad \beta_r = \beta_0 \alpha_r, \tag{5.2}$$

$$\beta_i = \alpha_i \beta_0 + \sum_{m=1}^{r-i} (\alpha_{i+m}\beta_m + \alpha_m \beta_{i+m}), \quad i = 1, 2, \ldots, r-1, \tag{5.3}$$

$$g_{ij} = \tfrac{d}{\beta^2} \sum_{m=0}^{r-i} (\alpha_{i+m}\beta_{j+m} + \alpha_{j+m}\beta_{i+m}), \quad j \leq i, i = 1, 2, \ldots, r, \tag{5.4}$$

$$D = (d), \qquad d \neq 0. \tag{5.5}$$

In accordance with the definition in [23], the method (5.1) is said to be symmetric if

$$\alpha_0 = \alpha_r = 1,\ \alpha_i = -\alpha_{r-i},\ \beta_j = \beta_{r-j},\ i = 1,2,\ldots,r-1,\ j = 0,1,\ldots,r, \tag{5.6}$$

i.e.

$$\rho(z) = -z^r\rho(1/z), \quad \sigma(z) = z^r\sigma(1/z), \tag*{(5.6)$'$}$$

where

$$\rho(z) = -\sum_{i=0}^{r-1}\alpha_{r-i}z^i + z^r, \quad \sigma(z) = \sum_{i=0}^{r}\beta_{r-i}z^i.$$

Let $\sigma(1) = \beta = 1$, $\rho(1) = 0$, Feng[5] has showed that the method (5.1) is linear symplectic iff (5.6)'(i.e. (5.6)) holds. It is clear that the symmetric method (5.1) satisfies (5.2) and (5.3). Therefore, the symmetric (or linear symplectic) OLMs are symplectic and preserve the quadratic invariants of the differential systems about the nonsingular matrix G given by (5.4). Some properties of the matrix G can been found in [23]. Eirola and Sanz-Serna have showed that the irreducible symmetric method (5.1) implies that G(or $\wedge$ in [23]) is nonsingular and proved that the symmetry of the method is necessary for conservation properties to hold about the nonsingular matrix G(or $\wedge$), but the following examples will show that (5.6) isn't necessary for (5.2) and (5.3). In fact, the following formulae (5.7) and (5.8) with the nonsingular matrix G are symmetric but (5.9) with the singular matrix G is not.

Example 5.1. For r=1, it follows from (5.2)-(5.5) that (5.1) is specialized to the canonical formula

$$y_n = y_{n-1} + hf(\beta_0(y_{n-1} + y_n)) \tag{5.7}$$

with $G = (\frac{d}{2\beta_0}), D = (d), \beta_0, d\neq 0$. Furthermore, (5.7) with $\beta_0 = 1/2$ is implicit midpoint formula

$$y_n = y_{n-1} + hf((y_{n-1} + y_n)/2).$$

Example 5.2. For r=2, it follows from (5.2)-(5.5) that

$$\beta_2 = \beta_0\alpha_2, \quad \beta_0(1-\alpha_2^2) = \beta_1\alpha_1, \quad \beta_1(1-\alpha_2) = \beta_0\alpha_1(1+\alpha_2).$$

Then (5.1) is specialized to one of the following two formulae.

$$(1)\quad y_n = y_{n-2} + hf(\beta_0(y_n + y_{n-2}) + \beta_1 y_{n-1}) \tag{5.8}$$

with $D = (d)$ and

$$G = \frac{d}{\beta^2}\begin{pmatrix} 2\beta_0 & \beta_1 \\ \beta_1 & 2\beta_0 \end{pmatrix},$$

where $\beta = 2\beta_0 + \beta_1 \neq 0$, $2\beta_0 \neq \beta_1$, $d \neq 0$, G is nonsingular.

$$(2)\quad y_n = (1-\alpha_2)y_{n-1} + \alpha_2 y_{n-2} + hf(\beta_0(y_n + (1+\alpha_2)y_{n-1} + \alpha_2 y_{n-2})) \tag{5.9}$$

with $D = (d)$ and

$$G = \frac{2d\beta_0}{\beta^2}\begin{pmatrix} 1 & \alpha_2 \\ \alpha_2 & \alpha_2^2 \end{pmatrix},$$

where $\beta = 2\beta_0(1+\alpha_2), d, \beta_0 \neq 0, |\alpha_2| \neq 1$, G is singular.

It is clear that (5.7)-(5.9) can preserve the quadratic invariant (2.4), but (5.9) is not symplectic, (5.7) and (5.8) are symplectic. This is in line with the conclusion by [23] that the symmetry (or linear symplecticity) of OLMs is sufficient and necessary for symplecticity.

6. Linear Two-Step Methods

Consider linear two-step methods[12]

$$y_n = \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + h(\beta_0 f(y_n) + \beta_1 f(y_{n-1}) + \beta_2 f(y_{n-2})) \tag{6.1}$$

with

$$\alpha_1 + \alpha_2 = 1,\ \alpha_1 + 2\alpha_2 = \beta_0 + \beta_1 + \beta_2,\ \alpha_1 + 4\alpha_2 = 2(\beta_1 + 2\beta_2).$$

The method (6.1) are of order 2 and can be writen equivalently in the form of the method (1.7) with

$$C_{11} = (\beta_0), C_{21} = (\beta_0, 0, 1, 0)^T, C_{12} = (\alpha_1, \alpha_2, \beta_1, \beta_2),$$

$$C_{22} = \begin{pmatrix} \alpha_1 & \alpha_2 & \beta_1 & \beta_2 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

It is easy to prove that the method (6.1) satisfying M=0 must be one of the following four formulae. The first is

$$y_n = y_{n-2} + h(\beta_0(f(y_n) + f(y_{n-2})) + 2(1-\beta_0) f(y_{n-1})) \tag{6.2}$$

with $D = (d)$ and

$$G = g_{11} \begin{pmatrix} 1 & \frac{\beta_0 - 1}{\beta_0} & \frac{-\beta_0^2 + 4\beta_0 - 2}{\beta_0} & \beta_0 - 1 \\ \frac{\beta_0 - 1}{\beta_0} & 1 & 1-\beta_0 & \beta_0 \\ \frac{-\beta_0^2 + 4\beta_0 - 2}{\beta_0} & 1-\beta_0 & \beta_0^2 & (1-\beta_0)\beta_0 \\ \beta_0 - 1 & \beta_0 & (1-\beta_0)\beta_0 & \beta_0^2 \end{pmatrix},$$

where $d = \frac{2(2\beta_0 - 1) g_{11}}{\beta_0}$, $\beta_0 \neq 0, 1/2$, $g_{11} \neq 0$. It is clear that G is singular.

The second is leap-frog formula (explicit midpoint)

$$y_n = y_{n-2} + 2hf(y_{n-1}) \tag{6.3}$$

with $D = (2g_{12}), g_{12} \neq 0$ and

$$G = \begin{pmatrix} 0 & g_{12} & 2g_{12} & 0 \\ g_{12} & 0 & 0 & 0 \\ 2g_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The third is the trapezoid formula

$$y_n = y_{n-1} + \frac{1}{2} h(f(y_{n-1}) + f(y_n)) \tag{6.4}$$

with $D = (1)$ and

$$G = \begin{pmatrix} 1 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The fourth is

$$y_n = 2y_{n-1} - y_{n-2} + h(\beta_0 f(y_n) + (\beta_0 - 1) f(y_{n-2}) + (1 - 2\beta_0) f(y_{n-1})) \tag{6.5}$$

with $D = (0)$ and

$$G = \begin{pmatrix} 1 & -1 & -\beta_0 & \beta_0 - 1 \\ -1 & 1 & \beta_0 & 1-\beta_0 \\ -\beta_0 & \beta_0 & \beta_0^2 & \beta_0(1-\beta_0) \\ \beta_0 - 1 & 1-\beta_0 & (1-\beta_0)\beta_0 & (\beta_0-1)^2 \end{pmatrix}.$$

For the four-formulae mentioned above, (6.2)-(6.4) are symmetric in accordance with the definition in [23] and linear symplectic. (6.2)-(6.5) are not symplectic, but preserve the quadratic invariant (2.4). Therefore, any linear two-step methods are not symplectic, but some of them are linear symplectc and preserve (2.4). This is in line with the conclusion by Tang[27] that there exists no symplectic LMMs for nonlinear Hamiltonian systems.

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