SYMPLECTIC DIFFERENCE SCHEMES FOR LINEAR HAMILTONIAN CANONICAL SYSTEMS ①②

线性哈密尔顿系统的辛差分格式

Abstract

In this paper, we present some results of a study, specifically within the framework of symplectic geometry, of difference schemes for numerical solution of the linear Hamiltonian systems. We generalize the Cayley transform with which we can get different types of symplectic schemes. These schemes are various generalizations of the Euler centered scheme. They preserve all the invariant first integrals of the linear Hamiltonian systems.

§1 Introduction

Recently, it becomes evident that the Hamiltonian formalism plays a fundamental role in mathematical physics. One needs only to recall a few examples: classical mechanics, quantum mechanics, hydrodynamics of a perfect fluid, plasma physics, and accelerator physics.

The evolution of Hamiltonian systems has the important property of being symplectic, i.e., the sum of the areas of the canonical variable pairs, projected on any two-dimensional surface in a phase space, is time invariant. In numerically solving these equations it is necessary to replace them with finite difference equations which preserve this symplectic evolution property. In [1] the first author proposed a systematic study of symplectic difference schemes for Hamiltonian systems from the viewpoint of symplectic geometry. We present here some developments for linear Hamiltonian systems.

An outline of this paper is as follows: Section 2 is devoted to a review of well known facts concerning symplectic structures and Hamiltonian mechanics. In Section 3 we review some properties of the symplectic matrix and the infinitesimal symplectic matrix. In Section 4 we review some linear symplectic difference schemes. Constructions of linear symplectic schemes based on the Padé approximation are described in §5. Generalized Cayley transform and its corresponding symplectic schemes and conservation laws are presented in §6.

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§2 Some Facts from Hamiltonian Mechanics and Symplectic Geometry

In this section we will review some facts from Hamiltonian mechanics and symplectic geometry which are fundamental to what follows. Consider the following system of differential equations on R^{2n}

$$\begin{aligned} \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i}, \\ \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i}, \end{aligned} \qquad i = 1, 2, ..., n \tag{2.1}$$

where $H(p, q)$ is some real valued smooth function on R^{2n}. We call (2.1) a canonical system of differential equations with Hamiltonian H. We denote $p_i = z_i$, $q_i = z_{i+n}$, $z = (z_1, \cdots, z_{2n})'$, and $\frac{\partial H}{\partial z} = (\frac{\partial H}{\partial z_1}, \cdots, \frac{\partial H}{\partial z_{2n}})' \in R^{2n}$. Then (2.1) becomes

$$\frac{dz}{dt} = J^{-1}\frac{\partial H}{\partial z} \tag{2.2}$$

with

$$J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}, \quad J' = -J = J^{-1} \tag{2.3}$$

where I_n is the identity matrix. The phase space R^{2n} is equipped with a standard symplectic structure defined by the "fundamental" differential 2-form

$$\omega = \sum_1^n dp_i \wedge dq_i.$$

Let g be a diffeomorphism of R^{2n}:

$$z = \begin{pmatrix} p \\ q \end{pmatrix} \to g(z) = \begin{bmatrix} g_1(z) \\ \vdots \\ g_{2n}(z) \end{bmatrix} = \begin{bmatrix} \hat{p}(p,q) \\ \hat{q}(p,q) \end{bmatrix}$$

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

$$\sum_1^n d\hat{p}_i \wedge d\hat{q}_i = \sum_1^n dp_i \wedge dq_i.$$

This is equivalent to the condition that

$$\left(\frac{\partial g}{\partial z}\right)' J \left(\frac{\partial g}{\partial z}\right) \equiv J$$

i.e. the Jacobian matrix $\dfrac{\partial g}{\partial z}$ is symplectic everywhere,

$$\frac{\partial g}{\partial z} = \begin{bmatrix} \frac{\partial \hat{p}}{\partial p} & \frac{\partial \hat{p}}{\partial q} \\ \frac{\partial \hat{q}}{\partial p} & \frac{\partial \hat{q}}{\partial q} \end{bmatrix}.$$

For every pair of smooth functions $H(z)$, $F(z)$ on R^{2n}, the Poisson bracket is defined as

$$\{H, F\} = \left(\frac{\partial H}{\partial z}\right)' J \left(\frac{\partial F}{\partial z}\right) = \left(\frac{\partial H}{\partial q}\right)' \frac{\partial F}{\partial p} - \left(\frac{\partial H}{\partial p}\right)' \frac{\partial F}{\partial q}.$$

The bracket operation is anti-symmetric, bilinear and satisfies the Jacobi identity. A function F on R^{2n} is called an invariant integral of the canonical system (2.2) with Hamiltonian H if

$$F(z(t)) = \text{const.}$$

independent of t for every solution $z(t)$ of (2.2). A necessary and sufficient condition for the above invariant is

$$\{H, F\} = 0.$$

The Hamiltonian H itself is an invariant integral of the system (2.2). The fundamental property of the canonical system (2.2) with Hamiltonian function H is that there exists a one parameter group of symplectic transformations $g^t = g_H^t$, called the phase flow of function H, such that the solution $z(t)$ of (2.2) with initial value $z(0)$ is given by

$$z(t) = g_H^t(z(0)).$$

So the time evolution of a Hamiltonian system is always symplectic.

§3 Some Properties of Symplectic Matrices

Let us now briefly sketch some properties of the symplectic matrix.

Definition 1. A matrix S of order $2n$ is called symplectic if it satisfies the relation

$$S'JS = J \tag{3.1}$$

where S' is the transpose of S. All symplectic matrices form a group $Sp(2n)$.

Definition 2. A matrix B of order $2n$ is called infinitesimal symplectic if

$$JB + B'J = 0. \tag{3.2}$$

All infinitesimal symplectic matrices form a Lie algebra $sp(2n)$ with commutation operation $[A, B] = AB - BA$, and $sp(2n)$ is the Lie algebra of Lie group $Sp(2n)$.

We have the following well-known propositions:

P1. $\det S = 1$, if $S \in Sp(2n)$

P2. $S^{-1} = -JS'J = J^{-1}S'J$, if $S \in Sp(2n)$

P3. $SJS' = J$, if $S \in Sp(2n)$

P4. Let

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where A, B, C, D are $n \times n$ matrices. Then $S \in Sp(2n)$ iff

$$AB' - BA' = 0, \quad CD' - DC' = 0, \quad AD' - BC' = I,$$
$$A'C - C'A = 0, \quad B'D - D'B = 0, \quad A'D - C'B = I.$$

P5. Matrices

$$\begin{pmatrix} I & B \\ 0 & I \end{pmatrix}, \quad \begin{pmatrix} I & 0 \\ D & I \end{pmatrix}$$

are symplectic if $B' = B$, $D' = D$.

P6. Matrix

$$\begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} \in Sp(2n) \quad \text{if} \quad A = (D')^{-1}.$$

P7. Matrix $S = M^{-1}N \in Sp(2n)$ iff $M'JM = N'JN$.

P8. Matrix

$$\begin{pmatrix} Q & I-Q \\ -(I-Q) & Q \end{pmatrix} \in Sp(2n) \quad \text{iff} \quad Q^2 = Q,\ Q' = Q.$$

P9. If $B \in sp(2n)$, then $\exp(B) \in Sp(2n)$.

P10. If $B \in sp(2n)$, and $|I+B| \neq 0$, then $F = (I+B)^{-1}(I-B) \in Sp(2n)$, the Cayley transform of B.

P11. If $B \in sp(2n)$, then $(B^{2m})'J = J(B^{2m})$.

P12. If $B \in sp(2n)$, then $(B^{2m+1})'J = -J(B^{2m+1})$.

P13. If $f(x)$ is an even polynomial and $B \in sp(2n)$, then $f(B')J = Jf(B)$.

P14. If $g(x)$ is an odd polynomial and $B \in sp(2n)$, then $g(B) \in sp(2n)$, i.e., $g(B')J + Jg(B) = 0$.

§4 Some Symplectic Schemes for Linear Hamiltonian Systems

A Hamiltonian system (2.1) is called linear if the Hamiltonian is a quadratic form of z

$$H(z) = \frac{1}{2}z'Cz, \quad C' = C,$$

and J is a standard antisymmetric matrix

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad J' = -J = J^{-1}, \quad \det J = 1.$$

Then the canonical system (2.1) becomes

$$\frac{dz}{dt} = Bz, \quad B = J^{-1}C, \quad C' = C, \tag{4.1}$$

where $B = J^{-1}C$ is infinitesimal symplectic. The solution of (4.1) is

$$z(t) = g^t z(0), \quad g^t = \exp(tB) \tag{4.2}$$

where g^t, as the exponential transform of infinitesimal symplectic tB, is symplectic (P.14).

Consider now a quadratic form $F(z) = \frac{1}{2}z'Az$. The Poisson bracket of two quadratic forms H, F is also a quadratic form

$$\{H, F\} = \frac{1}{2}z'(AJC - CJA)z.$$

The condition for the quadratic form F to be an invariant integral of the linear Hamiltonian system $\frac{dz}{dt} = J^{-1}Cz$ can be expressed in any one of the following equivalent ways:

$$F((\exp(tJ^{-1}C))z) \equiv F(z), \tag{4.3a}$$

$$\{H, F\} = 0, \tag{4.3b}$$

$$(\exp(tJ^{-1}C))'A(\exp(tJ^{-1}C)) = A, \tag{4.3c}$$

$$AJC = CJA. \tag{4.3d}$$

In [1] some types of the symplectic scheme are proposed. The first is called the time-centered Euler scheme

$$\frac{z^{n+1} - z^n}{\tau} = B\frac{z^{n+1} + z^n}{2}. \tag{4.4}$$

The transition $z^n \to z^{n+1}$ is given by the following

$$z^{n+1} = F_\tau z^n, \quad F_\tau = \phi(-\frac{\tau}{2}B), \quad \phi(\lambda) = \frac{1-\lambda}{1+\lambda}, \tag{4.5}$$

where F_τ, as the Cayley transform of infinitesimal symplectic $(-\frac{\tau}{2}B)$, is symplectic **(P10)**.

The second is the staggered explicit scheme for separable Hamiltonian. For a separable Hamiltonian

$$H(p,q) = \frac{1}{2}(p', q')S\begin{pmatrix} p \\ q \end{pmatrix} = \frac{1}{2}p'Up + \frac{1}{2}q'Vq \tag{4.6}$$

where

$$S = \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix},$$

$U' = U$ possitive definite and $V' = V$, the canonical equation (4.1) becomes

$$\begin{aligned} \frac{dp}{dt} &= -Vq, \\ \frac{dq}{dt} &= Up. \end{aligned} \tag{4.7}$$

The staggered explicit scheme is

$$\begin{aligned} \frac{1}{\tau}(p^{n+1} - p^n) &= -Vq^{n+\frac{1}{2}}, \\ \frac{1}{\tau}(q^{n+\frac{1}{2}+1} - q^{n+\frac{1}{2}}) &= Up^{n+1}. \end{aligned} \tag{4.8}$$

The $p's$ are set at integer times $t = n\tau$, and $q's$ at half-integer times $t = (n+\frac{1}{2})\tau$. The transition

$$w^n = \begin{bmatrix} p^n \\ q^{n+\frac{1}{2}} \end{bmatrix} \longrightarrow \begin{bmatrix} p^{n+1} \\ q^{n+\frac{1}{2}+1} \end{bmatrix} = w^{n+1}$$

is given by the following

$$w^{n+1} = F_\tau w^n,$$

where

$$F_\tau = \begin{bmatrix} I & 0 \\ -U & I \end{bmatrix}^{-1} \cdot \begin{bmatrix} I & -V \\ 0 & I \end{bmatrix} \tag{4.9}$$

as the product of two symplectic matrices is symplectic (**P5**), and has second order of accuracy.

§5 Construction of Symplectic Schemes Based on Padé Approximation

We know that the trajectory $z(t) = g^t z_0$ is the solution satisfying the initial condition $z(0) = z_0$. In a linear system g^t coincides with its own Jacobian. One might ask how the approximations of $\exp(tB)$ are. This is most simply described in terms of Padé rational approximations. Here we consider the rational approximation to $\exp(x)$ defined by

$$\exp(x) \sim \frac{n_{lm}(x)}{d_{lm}(x)} = g_{lm}(x) \tag{5.1}$$

where

$$n_{lm}(x)=\sum_{k=0}^{m}\frac{(l+m-k)!m!}{(l+m)!k!(m-k)!}(x)^k, \tag{5.2}$$

$$d_{lm}(x)=\sum_{k=0}^{l}\frac{(l+m-k)!l!}{(l+m)!k!(l-k)!}(-x)^k. \tag{5.3}$$

For each pair of nonnegative integers l and m, the Taylor's series expansion of $\dfrac{n_{lm}(x)}{d_{lm}(x)}$ about the origin shows that

$$\exp(x)-\frac{n_{lm}(x)}{d_{lm}}=o(|\ x\ |^{m+l+1}),\quad |x|\longrightarrow 0. \tag{5.4}$$

The resulting $(l+m)$-th order Padé approximation of $\exp(x)$ is denoted by g_{lm}.

Theorem 1. *Let B be an infinitesimal symplectic, then for sufficiently small $|t|$, $g_{lm}(tB)$ is symplectic iff $l=m$, i.e. $g_{ll}(x)$ is the (l,l) diagonal Padé approximant to* $\exp(x)$*.*

Proof. "If " part. Let $n_{ll}(x)=f(x)+g(x)$, $d_{ll}(x)=f(x)-g(x)$, where $f(x)$ is an even polynomial and $g(x)$ is an odd polynomial. In order to prove $g_{ll}(tB)\in Sp(2n)$, we need only to verify **(P7)**

$$(f(tB)+g(tB))'J(f(tB)+g(tB))=(f(tB)-g(tB))'J(f(tB)-g(tB)). \tag{5.5}$$

By (P.13,14), the L.H.S of (5.5) turns into

$$(f(tB')+g(tB'))J(f(tB)+g(tB))=J(f(tB)-g(tB))(f(tB)+g(tB)). \tag{5.6}$$

Similarly for the R.H.S., we have

$$(f(tB')-g(tB'))J(f(tB)-g(tB))=J(f(tB)+g(tB))(f(tB)-g(tB)). \tag{5.7}$$

Comparing (5.6) and (5.7) completes the proof of "If" part of the theorem.

"Only If" part. Without loss of generality, we may take $l>m$. We need only to notice that, in Proposition 7, the order of the polynomial on the right hand is higher than that on the left hand.

From Theorem 1, we can obtain a sequence of symplectic difference schemes based on the diagonal (k,k) approximant Padé table. For the (1.1) approximant, we have the Euler centered scheme (4.4).

$$z^{n+1}=z^n+\frac{\tau B}{2}(z^n+z^{n+1}),\quad F_\tau{}^{(1.1)}=\phi^{(1,1)}(\tau B),\quad \phi^{(1,1)}(\lambda)=\frac{1+\dfrac{\lambda}{2}}{1-\dfrac{\lambda}{2}}.$$

For the (2.2) approximant, we have

$$z^{n+1}=z^n+\frac{\tau B(z^n+z^{n+1})}{2}+\frac{\tau^2B^2}{12}(z^n-z^{n+1}), \tag{5.8}$$

its transition is

$$F_\tau{}^{(2.2)}=\phi^{(2,2)}(\tau B),\quad \phi^{(2.2)}(\lambda)=\frac{1+\dfrac{\lambda}{2}+\dfrac{\lambda^2}{12}}{1-\dfrac{\lambda}{2}+\dfrac{\lambda^2}{12}}. \tag{5.9}$$

Evidently this scheme has fourth-order accuracy. For (3.3), we get

$$z^{n+1} = z^n + \frac{\tau B}{2}(z^n + z^{n+1}) + \frac{\tau^2 B^2}{10}(z^n - z^{n+1}) + \frac{\tau^3 B^3}{120}(z^n + z^{n+1}), \tag{5.10}$$

$$F_\tau{}^{(3.3)} = \phi^{(3,3)}(\tau B), \ \phi^{(3.3)}(\lambda) = 1 + \frac{\lambda}{2} + \frac{\lambda^2}{10} + \frac{\lambda^3}{120} \Big/ \Big(1 - \frac{\lambda}{2} + \frac{\lambda^2}{10} - \frac{\lambda^3}{120}\Big). \tag{5.11}$$

This scheme has sixth order accuracy. For (4.4), we obtain

$$\begin{aligned} z^{n+1} =& z^n + \frac{\tau B}{2}(z^n + z^{n+1}) + \frac{3\tau^2 B^2}{28}(z^n - z^{n+1}) \\ &+ \frac{\tau^3 B^3}{84}(z^n + z^{n+1}) + \frac{\tau^4 B^4}{1680}(z^n - z^{n+1}), \end{aligned} \tag{5.12}$$

$$\begin{aligned} F_\tau{}^{(4.4)} =& \phi^{(4,4)}(\tau B), \\ \phi^{(4.4)}(\lambda) =& 1 + \frac{\lambda}{2} + \frac{3\lambda^2}{28} + \frac{\lambda^3}{84} + \frac{\lambda^4}{1680} \Big/ \Big(1 - \frac{\lambda}{2} + \frac{3\lambda^2}{28} - \frac{\lambda^3}{84} + \frac{\lambda^4}{1680}\Big). \end{aligned} \tag{5.13}$$

It has eighth order accuracy.

Theorem 2. *The difference schemes*

$$z^{k+1} = g_{ll}(\tau B) z^k, \quad l = 1, 2, 3, \cdots$$

for the system (4.2) *are symplectic of* $2l$*-th order accuracy.*

§6 Generalized Cayley Transformation and its Application

A matrix B is called non-exceptional if

$$\det(I + B) \neq 0. \tag{6.1}$$

We introduce a matrix S by

$$I + S = 2(I + B)^{-1} \tag{6.2}$$

with the inversion

$$I + B = 2(I + S)^{-1}. \tag{6.3}$$

S is likewise non-exceptional, and we have the Cayley transform[2]

$$S = (I - B)(I + B)^{-1} = (I + B)^{-1}(I - B), \tag{6.4}$$

$$B = (I - S)(I + S)^{-1} = (I + S)^{-1}(I - S). \tag{6.5}$$

Let A be an arbitrary matrix. The equation

$$S' A S = A \tag{6.6}$$

expresses the condition that the substitution of S into both variables z, w leaves invariant the bilinear form $z' A w$.

Lemma 1. *If the non-exceptional matrices B and S are connected by* (6.4) *and* (6.5), *and A is any matrix, then*

$$S' A S = A \tag{6.7}$$

iff

$$B' A + A B = 0. \tag{6.8}$$

Proof. Take the transpose of (6.5) one gets

$$I - S' = B'(I + S').$$

Multiplying on the right by AS and noting (6.6), one finds

$$A(S - I) = B'A(S + I)$$

and hence, multiplying $(S + I)^{-1}$ on the right one gets

$$-AB = B'A.$$

Conversely, if assuming (6.8) and multiply the transposed equation

$$S'(I + B') = I - B'$$

of (6.4) on the right by A, we have

$$S'A(I - B) = A(I + B)$$

which yields (6.7) on post-multiplication by $(I + B)^{-1}$.

Let $\phi(\lambda) = (1 - \lambda)/(1 + \lambda)$, then the Cayley transform of B is denoted by $\phi(B) = (I + B)^{-1}(I - B)$. By taking successively $A = J$ and $A = A'$ in Lemma 1, we get

Theorem 3. *The Cayley transform of a non-exceptional infinitesimal symplectic (symplectic) matrix is a non-exceptional symplectic (infinitesimal symplectic) matrix. Let $B = J^{-1}C$, $C' = C$, $B \in sp(2n)$, $det(I + \tau B) \neq 0$, $A' = A$. Then*

$$(\phi(\tau B))'A(\phi(\tau B)) = A \tag{6.9}$$

iff

$$B'A + AB = 0. \tag{6.10}$$

In other words, a quadratic form $F(z) = \frac{1}{2}z'Az$ is invariant under the symplectic transformation $\phi(\tau B)$ iff $F(z)$ is an invariant integral of the Hamiltonian system (4.1).

Theorem 4. *Let $\psi(\lambda)$ be a function of complex variable λ satisfying*

1° $\psi(\lambda)$ *is analytic with real coefficients in a neighborhood D of $\lambda = 0$.*

2° $\psi(\lambda)\psi(-\lambda) = 1$ *in D.*

3° $\psi_\lambda(0) \neq 0$. *Let A be a matrix of order $2n$. Then*

$$(\psi(\tau B))'A(\psi(\tau B)) = A \tag{6.11}$$

for all τ with sufficiently small $|\tau|$ iff

$$B'A + AB = 0. \tag{6.12}$$

Proof. The condition 2° implies $\psi^2(0) \neq 0$. So $\psi(0) \neq 0$. If

$$(\psi(\tau B))'A(\psi(\tau B)) = A$$

for all τ with sufficiently small $|\tau|$, then differentiating both sides of the above equation with respect to τ, we get

$$B'(\psi_\lambda(\tau B))'A\psi(\tau B) + (\psi(\tau B))'AB\psi_\lambda(\tau B) = 0.$$

Set $\tau = 0$, it becomes

$$(B'A + AB)\psi(0)\psi_\lambda(0) = 0,$$

i.e.

$$B'A + AB = 0.$$

Conversely, if $B'A + AB = 0$, then it is not difficult to verify that the equations

$$\psi_\lambda(\tau B')A = A\psi_\lambda(-\tau B), \quad \psi(\tau B')A = A\psi(-\tau B)$$

hold for any analytic function ψ. From condition 2° it follows that

$$\psi_\lambda(\lambda)\psi(-\lambda) - \psi(\lambda)\psi_\lambda(-\lambda) = 0,$$

so

$$\begin{aligned}\frac{d}{d\tau}(\psi(\tau B)'A\psi(\tau B)) &= \frac{d}{d\tau}(\psi(\tau B')A\psi(\tau B)) \\ &= B'\psi_\lambda(\tau B')A\psi(\tau B) + \psi(\tau B')AB\psi_\lambda(\tau B) \\ &= B'A\psi_\lambda(-\tau B)\psi(\tau B) + AB\psi(-\tau B')\psi_\lambda(\tau B) \\ &= (B'A + AB)\psi_\lambda(-\tau B)\psi(\tau B) = 0\end{aligned}$$

i.e. $\psi(\tau B')A\psi(\tau B) = \psi(0)A\psi(0) = A\psi^2(0) = A$. The proof is completed.

By taking successively $A = J$ and $A' = A$ in Theorem 4 and using (4.3) we get

Theorem 5. *Take $|\tau|$ sufficiently small so that τB has no eigenvalue at the pole of the function $\psi(\lambda)$ in Lemma 2. Then $\psi(\tau B) \in Sp(2n)$ iff $B \in sp(2n)$. Let $B = J^{-1}C$, $C' = C$, $A' = A$. Then*

$$(\psi(\tau J^{-1}C))'A(\psi(\tau J^{-1}C)) = A \tag{6.13}$$

iff

$$AJC = CJA. \tag{6.14}$$

In other words, a quadratic form $F(z) = \frac{1}{2}z'Az$ is invariant under the symplectic transformation $\psi(\tau B)$ iff $F(z)$ is an invariant integral of the system (4.1).

The transform $\psi(\tau B)$ based on Theorem 4 includes exponential transform $\exp(\tau B)$, Cayley transform $\phi(-\frac{\tau}{2}B)$ and diagonal Padé transform as special cases. Taking $\psi(\lambda)$ in Theorem 4 as a rational function, then necessarily $\psi(\lambda) = \dfrac{P(\lambda)}{P(-\lambda)}$, $P(\lambda)$ is a polynomial, and is often normalized by setting $P(0) = 1$, $P'(0) \neq 0$.

Theorem 6. *Let $P(\lambda)$ be a polynomial, $P(0) = 1$, $P'(0) \neq 0$, and*

$$\exp(\lambda) - \frac{P(\lambda)}{P(-\lambda)} = O(|\lambda|^{m+1}), \tag{6.15}$$

Then

$$P(-\tau B)z^{m+1} = P(\tau B)z^m,$$

i.e.

$$z^{m+1} = \frac{P(\tau B)}{P(-\tau B)}z^m \tag{6.16}$$

is a symplectic scheme of order m for the linear system (4.1). This difference scheme and the original system (4.1) have the same set of quadratic invariants.

In order to find rational approximants $\dfrac{P(x)}{P(-x)}$ to $\exp(x)$, we may express $\exp(x)$ in various ways. For example,

(1) $\exp(x) \sim \dfrac{n_{ll}(x)}{n_{ll}(-x)} = \dfrac{d_{ll}(-x)}{d_{ll}(x)}$, (2) $\exp(x) = 1 + \tanh\dfrac{x}{2}\Big/\Big(1 - \tanh\dfrac{x}{2}\Big)$,

(3) $\exp(x) = \dfrac{e^{\frac{x}{2}}}{e^{-\frac{x}{2}}}$, (4) $\exp(x) = \dfrac{1}{2}(1+e^{x})\Big/\Big(\dfrac{1}{2}(1+e^{-x})\Big)$.

Each denominator and numerator in the above expressions can be expanded about the origin in Taylor's series. The first term of the approximation gives the function $\psi(x) = (1+\frac{x}{2})/(1-\frac{x}{2})$ which yields the Euler centered scheme. Keeping $m(>1)$ terms in the expansions for both the denominator and numerator we will get function $\psi(x)$ which will extend the Euler centered schemes. The schemes obtained in this way are all symplectic schemes, however the order of accuracy of the first two kinds of schemes is higher than that of the last two kinds. For example, if in the formula (4) the first three terms of the expansions of the denominator and numerator are kept, then the 4-th order symplectic scheme is obtained. However, the same kind of truncation gives 6-th order schemes from (1) and (2).

References

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