Journal of Computational Mathematics, Vol.16, No.3, 1998, 193–202.

THE STEP-TRANSITION OPERATORS FOR MULTI-STEP METHODS OF ODE'S[*1)]

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Abstract

In this paper, we propose a new definition of symplectic multistep methods. This definition differs from the old ones in that it is given via the one step method defined directly on M which is corresponding to the m step scheme defined on M while the old definitions are given out by defining a corresponding one step method on $M \times M \times \cdots \times M = M^m$ with a set of new variables. The new definition gives out a steptransition operator $g : M \longrightarrow M$. Under our new definition, the Leap-frog method is symplectic only for linear Hamiltonian systems. The transition operator g will be constructed via continued fractions and rational approximations.

Key words: Multi-step methods, Explike and loglike function, Fractional and rational approximation, Simplecticity of LMM, Nonexistence of SLMM.

1. Introduction

The disadvantage of symplectic methods in using the information from past time steps leads to their needing more function evaluation than nonsymplectic methods. This disadvantage can be overcome if one could construct symplectic multi-step methods. But the first problem should be solved is to give out the definition of symplectic multi-step method. Until now, a popular idea is that an m-step method on M may be written as a one-step method on M^m. In paper [2, 7], the authors have investigated the circumstance under which a difference scheme can preserve the product symplectic structure on M^m. In this paper, a completely different criterion is given because the induced one-step method corresponding to the original multi-step method is defined, it gives out a transition operator $g : M \longrightarrow M$.

Consider the autonomous ODE's on R^n

$$\frac{dz}{dt} = a(z), \tag{1.1}$$

where $z = (z_1, \cdots, z_n)$ and $a(z) = (a_1(z), \cdots, a_n(z))$ is a smooth vector field on R^n defining the system. For equation (1.1), we define a linear m step method (LMM) in standard form by

$$\sum_{j=0}^{m} \alpha_j z_j = \tau \sum_{j=0}^{m} \beta_j a_j, \tag{1.2}$$

[*] Received December 15, 1995.

[1)] Prepared by Qin Mengzhao

where α_j and β_j are constants subject to the conditions

$$\alpha_m = 1, \quad |\alpha_0| + |\beta_0| \neq 0.$$

If $m = 1$, we call (1.2) a one step method. In other cases, we call it a multi-step method. Here linearity means the right hand of (1.2) linearly dependent on the value of $a(z)$ on integral points. For the compatibility of (1.2) with equation (1.1), it must at least of order one and thus satisfies

1°. $\alpha_1 + \alpha_2 + \cdots + \alpha_m = 0.$

2°. $\beta_0 + \beta_2 + \cdots + \beta_m = \sum_{j=0}^{m} j\alpha_j \neq 0.$

LMM method (1.2) has two characteristic polynomials

$$\zeta(\lambda) = \sum_{i=0}^{m} \alpha_i \lambda^i, \quad \sigma(\lambda) = \sum_{i=0}^{m} \beta_i \lambda^i. \tag{1.3}$$

Equation (1.2) can be written as

$$\zeta(E) y_n = \tau a(\sigma(E) y_n). \tag{1.4}$$

In section 2, we will study symplectic multi-step methods for linear Hamiltonian systems. We will give a new definition via transition operators which are corresponding to the multi-step methods. We will point out that if these operators are of exponential forms and their reverse maps are of Log forms then the original multi-step method are symplectic. In section 3, we will use continued fractions and rational approximations to approximate the transition operators. In section 4, we show that for non-linear Hamiltonian systems, there exists no symplectic multi-step methods in the sense of our new definition. Numerical examples are also presented.

2. Symplectic LMM for Linear Hamiltonian Systems

First we consider a linear Hamiltonian system

$$\frac{dz}{dt} = az, \tag{2.1}$$

where a is an infinitesimal $n \times n$ symplectic matrix. Its phase flow is $z(t) = \exp(ta) z_0$. The LMM for (2.1) is

$$\alpha_m z_m + \cdots + \alpha_1 z_1 + \alpha_0 z_0 = \tau a(\beta_m z_m + \cdots + \beta_1 z_1 + \beta_0 z_0). \tag{2.2}$$

Our goal is to find a matrix g, i.e., a linear transformation $g : R^{2n} \longrightarrow R^{2n}$ which can satisfy (2.2)

$$\alpha_m g^m(z_0) + \cdots + \alpha_1 g(z_0) + \alpha_0 z_0 = \tau a(\beta_m g^m(z_0) + \cdots + \beta_1 g(z_0) + \beta_0 z_0). \tag{2.3}$$

Such a map g exists for sufficiently small τ and can be represented by continued fractions and rational approximations. We call this transformation is step transition operator.

Definition 2.1. If g is a symplectic transformation, then we call its corresponding LMM (2.2) is symplectic.(We simply call it the method a SLMM.)

From (2.3), we have

$$\tau a = \frac{\alpha_0 I + \alpha_1 g^1 + \cdots + \alpha_m g^m}{\beta_0 I + \beta_1 g^1 + \cdots + \beta_m g^m}. \tag{2.4}$$

The characteristic equation for LMM is

$$\zeta(\lambda) = \tau\mu\sigma(\lambda), \tag{2.5}$$

where μ is the eigenvalue of the infinitesimal symplectic matrix a and λ is the eigenvalue of g.

Let

$$\psi(\lambda) = \frac{\zeta(\lambda)}{\sigma(\lambda)}, \tag{2.6}$$

then (2.5) can be written as

$$\tau\mu = \psi(\lambda). \tag{2.7}$$

It's reverse function is

$$\lambda = \phi(\tau\mu). \tag{2.8}$$

To study the symplecticity of the LMM, one only needs to study the properties of functions ϕ and ψ. We will see if ϕ is of the exponential form or ψ is of logarithmic form, the corresponding LMM is symplectic. We first study the properties of the exponential functions and logarithmic functions.

Explike and *Loglike* functions:

First we give out the properties of exponential functions

1°. $\exp(x)|_{x=0} = 1.$

2°. $\frac{d}{dx}\exp(x)|_{x=0} = 1.$

3°. $\exp(x+y) = \exp(x)\cdot\exp(y).$

If we substitute y by $-x$, we have

$$\exp(x)\exp(-x) = 1. \tag{2.9}$$

Definition 2.2. If function $\phi(x)$ satisfies $\phi(0) = 1, \phi'(0) = 1$ and $\phi(x)\phi(-x) = 1$, we call this function is an *explike* function.

It's well known, the inverse function of an exponential function is a logarithmic function $x \longrightarrow \log(x)$. It has the following properties

1°. $\log(x)|_{x=1} = 0.$

2°. $\frac{d}{dx}\log(x)|_{x=1} = 1.$

3°. $\log(xy) = \log(x) + \log(y).$

If we take $y = 1/x$, we get

$$\log(x) + \log\left(\frac{1}{x}\right) = 0. \tag{2.10}$$

Definition 2.3. If a function ψ satisfies $\psi(1)=0, \psi'(1)=1$ and

$$\psi(x)+\psi\Big(\frac{1}{x}\Big)=0, \tag{2.11}$$

we call it a *loglike* function.

Obviously, polynomials can not be explike functions or loglike functions, so we try to find explike and loglike functions in the form of rational functions.

Theorem 2.1[3]**.** *LMM is symplectic for linear Hamiltonian systems iff its step transition operator $g=\phi(\tau a)$ is explike, i.e., $\phi(\mu)\cdot\phi(-\mu)=1$, $\phi(0)=1, \phi'(0)=1$.*

Theorem 2.2[4]**.** *LMM is symplectic for linear Hamiltonian systems iff $\psi(\lambda)=\dfrac{\zeta(\lambda)}{\sigma(\lambda)}$ is a loglike function, i.e., $\psi(\lambda)+\psi\Big(\dfrac{1}{\lambda}\Big)=0$, $\psi(1)=0, \psi'(1)=1$.*

Proof. From Theorem 1, we have $\phi(\mu)\phi(-\mu)=1$, so $\lambda=\phi(\mu)$, $\dfrac{1}{\lambda}=\phi(-\mu)$. The inverse function of ϕ satisfies $\psi(\lambda)=\mu$, $\psi\Big(\dfrac{1}{\lambda}\Big)=-\mu$, i.e., $\psi(\lambda)+\psi\Big(\dfrac{1}{\lambda}\Big)=0$, $\psi(0)=1, \psi'(1)=1$ follows from consistency condition 1°, 2°.

On the other side, if $\psi(\lambda)=-\psi\Big(\dfrac{1}{\lambda}\Big)$, let $\psi(\lambda)=\mu$, then its inverse function is $\phi(\mu)=\lambda$ and $\phi(-\mu)=\dfrac{1}{\lambda}$, we then have $\phi(\mu)\phi(-\mu)=1$.

Theorem 2.3. *If $\xi(\lambda)$ antisymmetric polynomial, $\sigma(\lambda)$ is a symmetric one, then $\psi(\lambda)=\dfrac{\xi(\lambda)}{\sigma(\lambda)}$ satisfies*

$$\psi(1)=0, \quad \psi\Big(\frac{1}{\lambda}\Big)+\psi(\lambda)=0$$

Proof.

$$\tilde{\xi}(\lambda)=\lambda^m\xi\Big(\frac{1}{\lambda}\Big)=\sum_{i=0}^{m}\alpha_{m-i}\lambda^i=-\Sigma\alpha_i\lambda^i=-\xi(\lambda)$$

$$\tilde{\sigma}(\lambda)=\lambda^m\sigma\Big(\frac{1}{\lambda}\Big)=\sum_{i=0}^{m}\beta_{m-i}\lambda^i=\Sigma\beta_i\lambda^i=\sigma(\lambda)$$

$$\psi(\lambda)=\frac{\xi(\lambda)}{\sigma(\lambda)}, \quad \psi\Big(\frac{1}{\lambda}\Big)=\frac{\xi(\frac{1}{\lambda})}{\sigma(\frac{1}{\lambda})}=\frac{\lambda^m\xi(\frac{1}{\lambda})}{\lambda^m\sigma(\frac{1}{\lambda})}=-\frac{-\xi(\lambda)}{\sigma(\lambda)}$$

we obtain $\psi(\lambda)+\psi\Big(\dfrac{1}{\lambda}\Big)=0$. Now $\xi(1)=\displaystyle\sum_{k=0}^{m}\alpha_k=0$, $\sigma(1)=\displaystyle\sum_{k=0}^{m}\beta_u\neq 0$, then $\psi(1)=\dfrac{\xi(1)}{\sigma(1)}=0$.

Corollary 2.1. *If above generating polynomials is consistency with ODE* (1.1), *then $\psi(\lambda)$ is loglike function. i.e. $\psi\Big(\dfrac{1}{\lambda}\Big)+\psi(\lambda)=0$, $\psi(1)=0$, $\psi'(1)=1$.*

Proof. $\psi'(1)=\dfrac{\xi'\sigma-\sigma'\xi}{\sigma^2}=\dfrac{\xi'(1)}{\sigma(1)}=1$. This condition is not others just consistence condition.

Theorem 2.4. *Let* $\psi(\lambda) = \dfrac{\xi(\lambda)}{\sigma(\lambda)}$ *irreducible loglike function, then* $\xi(\lambda)$ *is an autisymmetric polynomial while* $\sigma(\lambda)$ *is a symmetric one.*

Proof. We write formally

$$\xi(\lambda) = \alpha_m\lambda^m + \alpha_{m-1}\lambda^{m-1} + \cdots \alpha_1\lambda + \alpha_0$$
$$\sigma(\lambda) = \beta_m\lambda^m + \beta_{m-1}\lambda^{m-1} + \cdots \beta_1\lambda + \beta_0$$

(if $\deg\xi(\lambda) = p < m$, set $a_i = 0$ for $i > p$, if $\deg Q(\lambda) = q < m$, set $\beta_i = 0$ for $i > q$). $\psi(1) = 0 \Longrightarrow \xi(1) = 0$, since otherwise, if $\xi(1) \neq 0$, then $\psi(1) = \dfrac{\xi(1)}{\sigma(1)} \neq 0$. Now $\xi(1) = 0 \Longleftrightarrow \sigma(1) \neq 0$, since otherwise $\xi(1) = \sigma(1) = 0 \Longrightarrow \xi(\lambda)$, $\sigma(\lambda)$ would have common factor. So we have

$$\xi(1) = \sum_{k=0}^{m}\alpha_k = \sum_{k=0}^{p}\alpha_k = 0, \qquad \sigma(1) = \sum_{k=0}^{m}\beta_k = \sum_{k=0}^{q}\beta_k \neq 0$$

If $m = \deg\xi = p$, then $\alpha_m = \alpha_p \neq 0$. If $m = \deg\sigma = q$, then $\beta_m = \beta_p \neq 0$

$$\psi\Big(\frac{1}{\lambda}\Big) = \frac{\xi(\frac{1}{\lambda})}{\sigma(\frac{1}{\lambda})} = \frac{\lambda^m\xi(\frac{1}{\lambda})}{\lambda^m\sigma(\frac{1}{\lambda})} = \frac{\tilde{\xi}(\lambda)}{\tilde{\sigma}(\lambda)}$$

Since $\psi(\lambda) + \psi\Big(\dfrac{1}{\lambda}\Big) = 0$, we have

$$\frac{\xi(\lambda)}{\sigma(\lambda)} = -\frac{\tilde{\xi}(\lambda)}{\tilde{\sigma}(\lambda)} \Longleftrightarrow \xi(\lambda)\tilde{\sigma}(\lambda) = -\tilde{\xi}(\lambda)\sigma(\lambda) \Longrightarrow \xi(\lambda) \mid \tilde{\xi}(\lambda)\sigma(\lambda), \quad \sigma(\lambda) \mid \tilde{\sigma}(\lambda)\xi(\lambda).$$

Since $\xi(\lambda)$, $\sigma(\lambda)$ have no common factor, then $\xi(\lambda) \mid \tilde{\xi}(\lambda)$, $\sigma(\lambda) \mid \tilde{\sigma}(\lambda)$. If $m = \deg\xi(\lambda) \Longrightarrow \deg\tilde{\xi} \leq \deg\xi \Longrightarrow \exists c$

$$\xi(\lambda) = c\tilde{\xi}(\lambda) \Longrightarrow \sigma(\lambda) = -c\tilde{\sigma}(\lambda)$$

Since $\alpha_m \neq 0 \Longrightarrow \alpha_m\lambda^m + \alpha_{m-1}\lambda^{m-1} + \cdots + \alpha_0 = c(\alpha_m + \cdots \alpha_0 w^m) \Longrightarrow \alpha_m = c\alpha_0$, $\alpha_0 = c\alpha_m \Longleftrightarrow \alpha_m = c^2\alpha_m$, therefore $c^2 = 1$, $c = \pm 1$. Suppose $c = +1$, then $\sigma(\lambda) = -\tilde{\sigma}(\lambda)$, $\sum_{r=0}^{m}\beta_k = \sigma(1) = -\tilde{\sigma}(1) = \sigma(1) \Longleftrightarrow \sigma(1) = 0$, this leads to a contradiction with the assumption $\sigma(1) \neq 0$. Therefore $c = -1$, i.e.

$$\xi(\lambda) = -\tilde{\xi}(\lambda), \quad \alpha_j = -\alpha_{m-j}, \quad j = 0, 1, \cdots, m$$
$$\sigma(\lambda) = \tilde{\sigma}(\lambda), \quad \beta_j = \beta_{m-j}, \quad j = 0, 1, \cdots, m$$

The proof for the case $m = \deg\sigma(\lambda)$ proceeds in exactly the same manner as above.

3. Rational Approximations to Exponential and Logarithmic Functions

1. We first study a simple example, the Leap-frog scheme

$$z_2 = z_0 + 2\tau a z_1. \tag{3.1}$$

Let $z_1 = cz_0$, then $z_0 = c^{-1}z_1$, insert this equation into (3.1), we get

$$z_2 = 2\tau a z_1 + \frac{1}{c}z_1 = \Big(2\tau a + \frac{1}{c}\Big)z_1 = d_1 z_1, \quad z_1 = \frac{1}{2\tau a + \frac{1}{c}}z_2 = \frac{z_2}{d_1},$$
$$z_3 = z_1 + 2\tau a z_2 = \Big(2\tau a + \cfrac{1}{2\tau a + \cfrac{1}{c}}\Big)z_2 = d_2 z_2, \quad z_2 = \frac{1}{2\tau a + \frac{1}{2\tau a + \frac{1}{c}}}z_3,$$
$$z_4 = \Big(2\tau a + \frac{1}{2\tau a + \frac{1}{2\tau a + \frac{1}{c}}}\Big) = d_4 z_3, \quad \cdots\cdots$$

where d_k can be written in the form of continued fractions

$$d_k = 2\tau a + \frac{1}{2\tau a +}\frac{1}{2\tau a +}\cdots\frac{1}{+\,2\tau a +}\cdots, \tag{3.2}$$

and

$$\lim_{k\to\infty} d_k = g = \tau a + \sqrt{1 + (\tau a)^2}. \tag{3.3}$$

We assume the transition operator of Leap-frog to be g, from (3.1) we have $g^2 - 1 = 2\tau a g$, now we have $g = \tau a \pm \sqrt{1 + (\tau a)^2}$. Here only sign + is meaningful, thus $g = \tau a + \sqrt{1 + (\tau a)^2}$ which is just the limit of continued fraction (3.2). It is easy to verify that g is explike, i.e., $g(\mu)g(-\mu) = 1$. So the Leap-frog scheme is symplectic for linear Hamiltonian systems in the sense our new definition.

2. For the exponential function

$$\exp(z) = 1 + \sum_{k=1}^{\infty}\frac{z^k}{k!}, \tag{3.4}$$

we have Lagrange's continued function

$$\begin{aligned}\exp(z) &= 1 + \frac{z}{1+}\,\frac{-z}{2}\,+\cdots+\frac{z}{2n-1+}\,\frac{-z}{2}\,+\cdots\\ &= b_0 + \frac{a_1}{b_1+}\,\frac{a_2}{b_2}\,+\cdots+\frac{a_{2n-1}}{b_{2n-1}+}\,\frac{a_{2n}}{b_{2n}}\,+\cdots,\end{aligned} \tag{3.5}$$

where

$$a_1 = z, \quad a_2 = -z, \quad \cdots, \quad a_{2n-1} = z, \quad a_{2n} = -z, \qquad n \ge 1,$$
$$b_0 = 1, \quad b_1 = 1, \quad b_2 = 2, \quad \cdots, \quad b_{2n-1} = 2n-1, \quad b_{2n} = 2, \qquad n \ge 1,$$

and Euler's contract expansion

$$\begin{aligned}\exp(z) &= 1 + \frac{2z}{2 - z +}\,\frac{z^2}{6}\,+\cdots+\frac{z^2}{2(2n-1)}\,+\cdots\\ &= B_0 + \frac{A_1}{B_1+}\,\frac{A_2}{B_2+}\,\cdots\,\frac{A_n}{+B_n}\,+\cdots,\end{aligned} \tag{3.6}$$

where

$$A_1 = 2z, \quad A_2 = z^2, \quad \cdots, \quad A_n = z^2, \qquad n \ge 2,$$

$$B_0 = 1, \quad B_1 = 2 - z, \quad B_2 = 6, \quad \cdots, \quad B_n = 2(2n-1), \qquad n \geq 2.$$

We have

$$\begin{aligned}
&\frac{P_0}{Q_0} = \frac{p_0}{q_0} = 1, \quad \frac{p_1}{q_1} = \frac{1+z}{1}, \quad \frac{p_2}{q_2} = \frac{P_1}{Q_1} = \frac{2+z}{2-z}, \quad \frac{p_3}{q_3} = \frac{6+4z+z^2}{6-2z} \\
&\frac{p_4}{q_4} = \frac{P_2}{Q_2} = \frac{12+6z+z^2}{12-6z+z^2} + \cdots
\end{aligned} \tag{3.7}$$

In general $p_{2n-1}(z)$ is a polynomial of degree n, q_{2n-1} is a polynomial of degree $n-1$, so p_{2n-1}/q_{2n-1} is not explike. While $p_{2n} = P_n(x)$, $q_{2n} = Q_n(z)$ are both polynomials of degree n and from the recursions

$$\begin{aligned}
&P_0 = 1, \quad P = 2 + z, \quad P_n = z^2 P_{n-2} + 2(2n-1)P_{n-1}, \\
&Q_0 = 1, \quad Q = 2 - z, \quad Q_n = z^2 Q_{n-2} + 2(2n-1)Q_{n-1}.
\end{aligned} \tag{3.8}$$

It's easy to see that for $n = 0, 1, \cdots$

$$Q_n(z) = P_n(-z), \quad P_n(0) > 0.$$

So the rational function

$$\phi_n(z) = \frac{P_n(z)}{Q_n(z)} = \frac{P_n(z)}{P_n(-z)}$$

is explike and

$$\phi_n(z) - \exp(z) = O(|z|^{2n+1}),$$

where

$$P_0 = 1, \quad P_1 = 2 + z, \quad P_n(z) = z^2 P_{n-2}(z) + 2(2n-1)P_{n-1}(z), \qquad n \geq 2. \tag{3.9}$$

This is just the diagonal Padé approximation.

3. For the logarithmic function

$$\log(w) = \sum_{k=1}^{\infty} \frac{(w-1)^k}{kw^k}, \tag{3.10}$$

we have the Lagrange's continued fraction

$$\begin{aligned}
\log(w) =& \frac{w-1}{1} + \frac{w-1}{2} + \frac{w-1}{3} + \frac{2(w-1)}{2} + \cdots + \frac{(n-1)(w-1)}{2n-1} + \frac{n(w-1)}{2} + \cdots \\
=& \frac{a_1}{b_1} + \frac{a_2}{b_2} + \frac{a_3}{b_3} + \frac{a_4}{b_4} + \cdots + \frac{a_{2n-1}}{b_{2n-1}} + \frac{a_{2n}}{b_{2n}} + \cdots,
\end{aligned} \tag{3.11}$$

where

$$\begin{aligned}
&a_1 = w-1, \ a_2 = w-1, \ a_3 = w-1, \ a_4 = 2(w-1), \cdots, \\
&b_0 = 0, \ b_1 = 1, \ b_2 = 2, \ b_3 = 3, \ b_4 = 2, \ \cdots,
\end{aligned}$$

and

$$a_{2n-1} = (n-1)(w-1), \ a_{2n} = n(w-1), \quad n \geq 2,$$

$$b_{2n-1} = 2n-1,\ b_{2n} = 2, \quad n \geq 2,$$

and the Euler's contracted expansion

$$\begin{aligned}\log(w) =& \frac{2(w-1)}{w+1} - \frac{2(w-1)}{6(w+1)} - \frac{(2.2(w-1))^2}{2.5(w+1)} - \cdots - \frac{(2(n-1)(w-1))^2}{2(2n-1)(w+1)} - \cdots \\ =& \frac{A_1}{B_1} + \frac{A_2}{B_2} + \frac{A_3}{B_3} + \cdots + \frac{A_n}{B_n} + \cdots,\end{aligned} \tag{3.12}$$

where

$$\begin{aligned}&A_1 = 2(w-1),\ A_2 = -2(w-1),\ \cdots,\ A_n = -(2(n-1)(w-1))^2,\ n \geq 3,\\ &B_0 = 0,\ B_1 = w+1,\ B_2 = 6(w+1),\ \cdots,\ B_n = 2(2n-1)(w+1),\ n \geq 2.\end{aligned}$$

The followings can be get by recursion

$$\begin{aligned}&\frac{P_0}{Q_0} = \frac{p_0}{q_0} = 0,\ \frac{p_1}{q_1} = w-1,\ \frac{p_2}{q_2} = \frac{P_1}{Q_1} = \frac{2(w-1)}{w+1},\\ &\frac{p_3}{q_3} = \frac{w^2+4w-5}{4w+2},\ \frac{p_4}{q_4} = \frac{P_2}{Q_2} = \frac{3(w^2-1)}{w^2+4w+1}, \cdots.\end{aligned} \tag{3.13}$$

In general

$$\frac{p_{2n-1}(w)}{q_{2n-1}(w)} - \log(w) = O(|w-1|^{2n}), \quad \frac{p_{2n}(w)}{q_{2n}(w)} - \log(w) = O(|w-1|^{2n+1}).$$

The rational function $\frac{p_{2n-1}(w)}{q_{2n-1}(w)}$ approximates $\log(w)$ only by odd order $2n-1$, it does not reach the even order $2n$, and is not loglike. However

$$R_n = \psi_n(w) = \frac{p_{2n}(w)}{q_{2n}(w)} = \frac{P_n(w)}{Q_n(w)}$$

is a loglike function. In fact, by recursion, it's easy to see that

$$P_n(w) = -w^n P_n\Big(\frac{1}{w}\Big), \quad Q_n(w) = w^n Q_n\Big(\frac{1}{w}\Big), \tag{3.14}$$

and $\forall n$, $Q_n(1) \neq 0$. We also have

$$\begin{aligned}&P_0 = 0,\ P_1(w) = 2(w-1),\ P_2(w) = 3(w^2-1),\\ &Q_0 = 1,\ Q_1(w) = w+1,\ Q_2(w) = w^2+4w+1,\end{aligned}$$

and for $n \geq 3$,

$$\begin{aligned}P_n(w) &= -(2(n-1)(w-1))^2 P_{n-2}(w) + 2(2n-1)(w-1)P_{n-2}(w),\\ Q_n(w) &= -((2n-1)(w-1))^2 Q_{n-2}(w) + 2(2n-1)(w-1)Q_{n-2}(w).\end{aligned} \tag{3.15}$$

So we see $R_1(\lambda)$ is just the Euler midpoint rule and $R_2(\lambda) = \frac{3(\lambda^2-1)}{\lambda^2+4\lambda+1}$ is just the Simpson scheme.

Conclusion: The odd truncation of the continued fraction of the Lagrange's approximation to $\exp(x)$ and $\log(x)$ is not explike nor loglike, while the even truncation is explike and loglike. The truncation of the continued fraction got from Euler's contracted expansion is explike and loglike.

4. Another famous rational approximation to a given function is the Obreschkoff formula[8],

$$\begin{aligned} R_{m,n}(x) : \sum_{k=0}^{n} \frac{c_n^k}{c_{m+n}^k k!}(x_0 - x)^k f^{(k)}(x) - \sum_{k=0}^{m} \frac{c_m^k}{c_{m+n}^k k!}(x - x_0)^k f^{(k)}(x_0) \\ = \frac{1}{(m+n)!} \int_{x_0}^{x} (x-t)^m (x_0 - t)^n f^{(m+n+1)}(t)\ dt. \end{aligned} \tag{3.16}$$

1°. Take $f(x) = e^x, x_0 = 0$, we obtain Padé approximation $\exp(x) \doteq R_{m,n}(x)$. If $m = n$, we obtain Padé diagonal approximation $R_{m,m}(x)$.

2°. Take $f(x) = \log(x), x_0 = 1$, we obtain $\log(x) \doteq R_{m,n}(x)$. If $m = n$, we obtain loglike function $R_m(x)$,

$$R_m(\lambda) = \frac{1}{\lambda^m} \sum_{k=1}^{m} \frac{c_m^k}{c_{2m}^k k}(\lambda - 1)^k (\lambda^{m-k} + (-1)^{k-1}\lambda^m),$$

i.e.,

$$R_m(\lambda) + R_m\Big(\frac{1}{\lambda}\Big) = 0.$$

We have

$$\begin{aligned} &R_m(\lambda) - \log(\lambda) = O(|\lambda|^{2n+1}), \\ &R_1 = \frac{\lambda^2 - 1}{2\lambda}, \\ &R_2(\lambda) = \frac{1}{12\lambda^2}(-\lambda^4 + 8\lambda^3 - 8\lambda + 1), \\ &R_3(\lambda) = \frac{1}{60\lambda^3}(\lambda^6 - 9\lambda^5 + 45\lambda^4 - 45\lambda^2 + 9\lambda - 1), \\ &\quad \cdots\cdots \end{aligned}$$

where $R_1(\lambda)$ is just the leap-frog scheme.

4. Nonexistence of SLMM for Nonlinear Hamiltonian Systems

For nonlinear Hamiltonian systems, there exists no symplectic LMM. When equation (1.1) is nonlinear, how to define a symplectic LMM? The answer is to find the step-transition operator $g : R^n \longrightarrow R^n$, let

$$\begin{aligned} &z = g^0(z), \\ &z_1 = g(z), \\ &z_2 = g(g(z)) = g \circ g(z) = g^2(z), \\ &\quad \cdots\cdots \end{aligned} \tag{4.1}$$

$$z_n = g(g(\cdots(g(z))\cdots) = g \circ g \circ \cdots \circ g \circ z) = g^n(z),$$

we get from (1.2)

$$\sum_{i=0}^{k} \alpha_i g^i(z) = \tau \sum_{i=0}^{n} \beta_i f \circ g^i(z). \tag{4.2}$$

It's easy to prove that if LMM (4.2) is consistent with equation (1.1), then for smooth f and sufficiently small step-size τ, the operator g defined by (4.1) exists and it can be represented as a power series in $\tau$and is near identity. Consider the case that equation (1.1) is an Hamiltonian system, i.e., $a(z) = J\nabla H(z)$, we have the following definition.

Definition 4.4. LMM is symplectic if the trsnsition operator g defined by (4.1) is symplectic for all $H(z)$ and all step-size τ, i.e.,

$$g_*(z)' J g_*(z) = J. \tag{4.3}$$

This definition is a completely different criterion that can include the symplectic condition for one-step methods in the usual sense. But Tang in [5] has proven that non linear multistep method can satisfy such a strict criterion. Numerical experiments due to Li in [6] shows the explicit 3-level centered method(Leap-frog method) is symplectic for linear Hamiltonian systems $H = \frac{1}{2}(p^2 + 4q^2)$(See Fig 1 of [6]) but is non-symplectic for nonlinear Hamiltonian system $H = \frac{1}{2}(p^2 + q^2) + \frac{2}{3}q^4$(See Fig 2(a,b) of [6]).

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