Journal of Computational Mathematics, Vol.12, No.3, 1994, 235–238.

SYMPLECTIC MULTISTEP METHODS FOR LINEAR HAMILTONIAN SYSTEMS *1)

Li Wang-yao
(*Computing Center, Academia Sinica, Beijing, China*)

Abstract

Three classes of symplectic multistep methods for linear Hamiltonian systems are constructed and their stabilities are discussed in this paper.

1. Introduction

Professor Feng Kang advanced the principle for construction of symplectic algorithms for Hamiltonian systems[1] and pointed out, that symplectic algorithms can reflect main features of Hamiltonian systems, therefore they are more available. Plenty of theoretical and numerical results have proved these points.

Professor Feng Kang also discussed the approximation problems by algebraic functions. The conclusions are stated as follows[2]:

1. We note $\psi(\xi)=\rho(\xi)/\sigma(\xi)$. A multistep method $M(\rho,\sigma)$ is symplectic for linear Hamiltonian systems (we call it linear symplectic for short) iff $\psi(\xi)=-\psi(1/\xi)$.

2. Assume ρ and σ have no common factor. $\rho(\xi)$ is antisymmetric ($\xi^K\rho(1/\xi)=-\rho(\xi)$) and $\sigma(\xi)$ is symmetric ($\xi^K\sigma(1/\xi)=\sigma(\xi)$) iff $\psi(\xi)=-\psi(1/\xi)$.

Dased on the above results, in this paper three classes of linear symplectic multistep formulas are given and some good proterties are discussed.

2. The Construction of Linear Symplectic Multistep Formulae

Lemma 1. *All roots of $\rho(\xi)$ have module equal to unit and are simple if the linear multistep formulae $M(\rho,\sigma)$ are linear symplectic.*

Proof. According to symplectic condition $\psi(\xi)=-\psi(1/\xi)$ if ξ is a root of $\rho(\xi)$, so does $1/\xi$. The module of no root of $\rho(\xi)$ is exceeds 1 and the roots of module 1 are simple (stability condition), therefore lemma 1 holds.

Lemma 2. *$\rho(\xi)$ is antisymmetric if* $\rho(\xi)=(\xi-1)(\xi+1)(\xi-e^{i\varphi_1})(\xi-e^{-i\varphi_1})\cdots(\xi-e^{i\varphi_P})(\xi-e^{-i\varphi_P})$.

* Received May 3, 1993.

1) The Project Supported by National Natural Science Foundation of China.

Proof. Since $\xi(1/\xi - 1) = -(\xi - 1)$, $\xi(1/\xi + 1) = (\xi + 1)$ and

$$\xi^2(1/\xi - e^{i\varphi})(1/\xi - e^{-i\varphi}) = (1 - \xi e^{i\varphi})(1 - \xi e^{-i\varphi}) = (\xi - e^{i\varphi})(\xi - e^{-i\varphi}),$$

we have

$$\xi^{2(p+1)}\rho(1/\xi) = -\rho(\xi).$$

When

$$\rho(\xi) = (\xi - 1)(\xi - e^{i\varphi_1})(\xi - e^{-i\varphi_1})\cdots(\xi - e^{i\varphi_p})(\xi - e^{-i\varphi_p}),$$

the proof is the same.

Theorem 1. *$\rho(\xi)$ stands for above mentioned antisymmetric polynomial of degree k. If k is even, then the only symmetric polynomial $\sigma(\xi)$ of degree k can be defined, so that the linear symplectic implicit k-step formulae $M(\rho, \sigma)$ have order $k+2$. (i.e. optimal methods). If k is odd, then the only symmetric polynomial $\sigma(\xi)$ of degree k can be defined, so that the linear symplectic implicit k-step formulae $M(\rho, \sigma)$ have order $k+1$.*

Proof. Let

$$\xi = \frac{1+z}{1-z}, \qquad z = \frac{\xi - 1}{\xi + 1}$$

and

$$r(z) = \Big(\frac{1-z}{2}\Big)^K \rho\Big(\frac{1+z}{1-z}\Big), \qquad s(z) = \Big(\frac{1-z}{2}\Big)^K \sigma\Big(\frac{1+z}{1-z}\Big).$$

$r(z)$ is odd function because

$$r(-z) = \Big(\frac{1+z}{2}\Big)^K \rho\Big(\frac{1-z}{1+z}\Big) = -\Big(\frac{1+z}{2}\Big)^K \Big(\frac{1-z}{1+z}\Big)^K \rho\Big(\frac{1+z}{1-z}\Big)$$
$$= -\Big(\frac{1-z}{2}\Big)^K \rho\Big(\frac{1+z}{1-z}\Big) = -r(z).$$

It is well known that the multistep method $M(\rho, \sigma)$ has order p if and only if $P(z) = r(z)/\log(\frac{1+z}{1-z}) - s(z)$ has a zero of order p at z=0 (see Henrici [3]). We choose the k terms in front of Taylor series of $r(z)/\log(\frac{1+z}{1-z})$ as s(z), then the multistep method $M(\rho, \sigma)$ associated with r(z) and s(z) has order k+1. Both $r(z)$ and $\log((1+z)/(1-z))$ are odd, so s(z) is even. According to this, $\sigma(\xi)$ is symmetric and $M(\rho, \sigma)$ has order k+2 when k is even.

Theorem 2. *$\rho(\xi)$ stands for above mentioned antisymmetric polynomial of degree k. If k is even, then a symmetric polynomial $\sigma(\xi)$ of degree k can be defined, so that the linear symplectic explicit k-step formulae $M(\rho, \sigma)$ have order k.*

Proof. For optimal methods $\sigma(\xi)$ may express as

$$\sigma(\xi) = C_0\xi^{k/2} + C_1\xi^{k/2-1}(\xi - 1)^2 + \cdots + C_{k/2}(\xi - 1)^k \tag{1}$$

where C_i is a definite constant. If the last term $C_{k/2}(\xi - 1)^k$ in (1) is taken away, $\sigma(\xi)$ is a symmetric polynomial of degree $k-1$ and the corresponding linear symplectic k-step formulae are explicit and of order k. (see [3]).

Example. 1. Implicit linear symplectic k (even)-step methods of order $k+2$ (optimal methods):

$k=2, y_{n+2}-y_n=h(2f_{n+1}-\frac{1}{3}\nabla^2 f_{n+2})$, Milne-Simpson formula;

$k=4, y_{n+4}-y_n=h(4f_{n+2}+\frac{8}{3}\nabla^2 f_{n+3}+\frac{14}{45}\nabla^4 f_{n+4})$;

$k=6, y_{n+6}-y_{n+5}+y_{n+4}-y_{n+2}+y_{n+1}-y_n=h(4f_{n+3}+\frac{20}{3}\nabla^2 f_{n+4}+\frac{134}{45}\nabla^4 f_{n+5}$ $+\frac{286}{675}\nabla^6 f_{n+6})$.

2. Explicit linear symplectic k(even)-step methods of order k :

$k=2, y_{n+2}-y_n=2hf_{n+1}$, Leap-frog formula;

$k=4, y_{n+4}-y_n=h(4f_{n+2}+\frac{8}{3}\nabla^2 f_{n+3})$;

$k=6, y_{n+6}-y_{n+5}+y_{n+4}-y_{n+2}+y_{n+1}-y_n=h\Big(4f_{n+3}+\frac{20}{3}\nabla^2 f_{n+4}+\frac{134}{45}\nabla^4 f_{n+5}\Big)$.

3. Implicit linear symplectic k(odd)-step methods of order $k+1$:

$k=1, y_{n+1}-y_n=\frac{h}{2}(f_{n+1}+f_n)$, Trapeizoid formula;

$k=3, y_{n+3}-y_{n+2}+y_{n+1}-y_n=\frac{h}{12}(5f_{n+3}+7f_{n+2}+7f_{n+1}+5f_n)$.

3. Some Properties of Linear Symplectic Multistep Methods

For the test problem $y'=\lambda y$, the characteristic equation of $M(\rho,\sigma)$ is

$$\psi(\xi)=\mu, \tag{2}$$

where

$$\psi(\xi)=\rho(\xi)/\sigma(\xi), \quad \mu=\lambda h.$$

Lemma 3. *The characteristic equation (2) corresponding to linear symplectic multistep formula $M(\rho,\sigma)$ maps the circle $|\xi|=1$ on the ξ-plane onto a segment on the imaginary axis of μ-plane which is symmetric to $\mu=0$.*

Proof. Because $\psi(e^{i\varphi})=-\psi(e^{-i\varphi})=-\bar{\psi}(e^{i\varphi})$ and $\psi(0)=0$, lemma 3 holds.

Theorem 3. *There exists a interval D: $[-ih,ih]$ on the imaginary axis of μ-plane such that all roots of the characteristic equation (2) of linear symplectic multistep formulae $M(\rho,\sigma)$ lie on the circle $|\xi|=1$ as long as $\mu=h\lambda\in D$.*

Proof. The roots of $\rho(\xi)$ divide the circle $|\xi|=1$ into k arcs (as shown in figure 1). When ξ moves along the circle from $\xi=1$ to the second zero of ρ, μ moves along the imaginary axis from $\mu=0$ to $h1$ (or infinity) and then return to $\mu=0$. Moreover, ξ continue to move from second zero to third zero, μ moves once again from $\mu=0$ to $h2$, then return to $\mu = 0$. Due to symmetry there are the same drawing on the half plane im $\xi < 0$ and im $\mu < 0$.

Therefore, all eigenvalues (there are four eigenvalues in figure 1) lie on the circle $|\xi| = 1$ if $h = \min(h1, h2)$ and $\mu \in [-ih, ih]$.

This proof is available to other more complicated situation.

Remark. If linear Hamiltonian systems only have imaginary eigenvalues, so it's basic solutions are periodic, Correspodingly, the numerical solutions by linear symplectic multistep methods also have periodicity when $h\lambda = \mu \in [-ih, ih]$.

Theorem 4. *There does not exist above mentioned interval $D : [-ih, ih]$ in linear multistep methods except linear symplectic multistep methods.*

Proof. If there exist infinite number of φ for linear multistep methods $M(\rho, \sigma)$ so that $\psi(e^{i\varphi}) = \rho(e^{i\varphi})/\sigma(e^{i\varphi}) = iy$, $\psi(e^{i\varphi}) = -\psi(e^{-i\varphi})$ hold for infinite number of φ, then, we have $\psi(\xi) = -\psi(1/\xi)$, i.e., the method is linear symplectic. For non-symplectic multistep methods, $\psi(\xi)$ only maps finite number of ξ on the the circle $|\xi| = 1$ onto imaginary axis so there does not exist above mentioned interval D.

References

[1] Feng Kang, On difference schemes and symplectic geometry, Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations.

[2] Feng Kang, On approximation by algebraic functions, Proceeding of the Annual Meeting on Computational Matematics in Tianjin, China, 1990.

[3] Peter Henrici, Discrete Variable Methods in Ordinary Differential Equations, John Wiley & Sons, Inc., New York, London.