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EXPLICIT SYMPLECTIC DIFFERENCE SCHEMES FOR SEPARABLE HAMILTONIAN SYSTEMS*1)

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Abstract

This paper is to develop explicit fourth order symplectic difference schemes for separable Hamiltonian systems.

§1. Introduction

In DD5 Beijing conference, Feng Kang [1] proposed an approach for computing Hamiltonian equations from the viewpoint of symplectic geometry. The theory of symplectic difference schemes of Hamiltonian systems and the methods of constructing symplectic difference schemes via generating functions are systematically developed in [1–6]. Symplectic difference schemes preserve the "symplecticity", i.e. the "canonicity" of the phase flow as well as the quadratic first integrals of the original Hamiltonian systems. All such schemes are implicit in principle. However, for the case of "separable" Hamiltonian $H(p,q) = U(p) + V(q)$, practically explicit symplectic schemes are possible as discussed in [1, 2, 3, 6] in which a first order explicit symplectic scheme and a second order time–staggered explicit symplectic scheme are given. In [7], a third order explicit symplectic scheme for separable Hamiltonians is proposed. In this paper, we construct fourth order explicit symplectic difference schemes by the algebraic method.

§2. Some Facts of Hamiltonian Mechanics

In this section we consider the Hamiltonian for relativistic motion

$$H(p,q,t) = g(p) + v(q,t). \tag{2.1}$$

In that case

$$g(p) = \sqrt{\langle p,p\rangle + m^2c^2} \tag{2.2}$$

where $p = (p_1, \cdots, p_n)^T, q = (q_1, \cdots, q_n)^T$ are n–dimensional vectors. The superscript T represents matrix transpose. The equations of motion can then be written in terms of Hamilton's equations

$$\frac{dp}{dt} = -\frac{\partial H(p,q,t)}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial H(p,q,t)}{\partial p}. \tag{2.3}$$

This system is a nonautonomous Hamiltonian system.

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An approach, which applies particularly to nonautonomous systems, is to regard the time t as an additional dependent variable. That is, letting $q_{n+1} = t$, we can choose a parameter τ as a new independent variable. It is well known [8, 9] that

$$p_{n+1} = -H,$$

which has a unit of energy, is the generalized momentum conjugate to the time t.

The function $K(w)$ where $w = (q_1, q_2, \cdots, q_n, t, p_1, p_2, \cdots, p_n, -H)^T$ takes place of the Hamiltonian function H; hence we shall call it the *extended Hamiltonian function*. The corresponding *extended Hamiltonian system* is

$$\frac{dz}{d\tau} = J^{-1}K_w(w), \qquad J = \begin{bmatrix} 0 & I_{n+1} \\ -I_{n+1} & 0 \end{bmatrix}. \tag{2.4}$$

In other words, the canonical equations become

$$\frac{dp_i}{d\tau} = -\frac{\partial K}{\partial q_i}, \quad \frac{dq_i}{d\tau} = \frac{\partial K}{\partial p_i}, \qquad i = 1, 2, \cdots, n+1. \tag{2.5}$$

For the special choice $K = p_{n+1} + H(q_1, \cdots, q_n, q_{n+1}, p_1, \cdots, p_n)$, we have

$$\frac{dp_i}{d\tau} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{d\tau} = \frac{\partial H}{\partial p_i}, \qquad i = 1, 2, \cdots, n, \tag{2.6}$$

$$\frac{dp_{n+1}}{d\tau} = -\frac{\partial H}{\partial q_{n+1}}, \tag{2.7}$$

$$\frac{dq_{n+1}}{d\tau} = 1. \tag{2.8}$$

Equation (2.8) shows that our normalized parameter τ is equal to q_{n+1} which is the time t. Equations (2.6) are the original canonical equations. Equation (2.7) shows that the negative of the total energy p_{n+1} changes with the time t.

We notice that after the time t is added to the mechanical variables, every system becomes autonomous. The extended Hamiltonian function K does not depend on variable τ explicitly. Thus the corresponding system is autonomous Hamiltonian in the extended phase space.

From the above consideration, we have

Proposition 2.1. For nonautonomous separable Hamiltonian (2.1), introducing new variables $q_{n+1} = t, p_{n+1} = -H$ yields an autonomous separable Hamiltonian system.

In order to construct an explicit symplectic difference scheme for Hamiltonian system (2.3) with the separable Hamiltonian (2.1), it is sufficient to construct an explicit symplectic difference scheme for the autonomous Hamiltonian system (2.4) or for the following form

$$\frac{dp}{dt} = -H_q(p, q) \equiv f(q), \quad \frac{dq}{dt} = H_p(p, q) \equiv g(p). \tag{2.10}$$

§3. Construction of Explicit Multi-Step Symplectic Difference Schemes

A four-step explicit method is defined by

$$p_1 = p_0 + c_1 h f(q_0), \qquad q_1 = q_0 + d_1 h g(p_1), \tag{3.1}$$