CONSTRUCTION OF CANONICAL DIFFERENCE SCHEMES FOR HAMILTONIAN FORMALISM VIA GENERATING FUNCTIONS * 1)

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Abstract

This paper discusses the relationship between canonical maps and generating functions and gives the general Hamilton-Jacobi theory for time-independent Hamiltonian systems. Based on this theory, the general method–*the generating function method*–of the construction of difference schemes for Hamiltonian systems is considered. The transition of such difference schemes from one time-step to the next is canonical. So they are called the canonical difference schemes. The well known Euler centered scheme is a canonical difference scheme. Its higher order canonical generalisations and other families of canonical difference schemes are given. The construction method proposed in the paper is also applicable to time-dependent Hamiltonian systems.

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§0. Introduction

As is well known, Hamiltonian systems have many intrinsic properties: the preservation of phase areas of even dimension and the phase volume, the conservation laws of energy and momenta and other symmetries. The *canonicity* of the phase flow for time-independent Hamiltonian systems is the most important property. It

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ensures the preservation of phase areas and the phase volume. Thus we can hope that preserving the canonicity of transition of difference schemes from one time step to the next is also important in numerical solution of Hamiltonian systems. The first author in [1] has proposed a notion–*canonical difference schemes*. Just as its name implies, the transition of such difference schemes is canonical. In this paper, we give a general method –*generating function method*–for the construction of canonical difference schemes via generating functions. We first establish the relationship between canonical maps and generating functions and then give the general Hamilton–Jacobi theory for time–independent Hamiltonian systems. Given a matrix $\alpha \in \mathrm{CSp}(\tilde{J}_{4n}, J_{4n})$, then canonical maps and generating functions can be determined each other under so called transversality conditions. Moreover, to the phase flow of the system with Hamiltonian H there corresponds a time-dependent generating function which satisfies the Hamilton-Jacobi equation related to the given α and H. If the Hamiltonian function is analytic, then the generating function can be expressed as a power series in t, and the series can be determined recursively(Theorem 20). So truncating or approximating it in some way, we can get certain canonical map which approximates the phase flow of the Hamiltonian system. Fixing t as the time step, we obtain difference schemes. In general, such difference scheme is implicit.

In Sec. 1, we review some notions and facts about symplectic geometry which can be found in the standard texts, e.g., [2], [3], [4]. Sec. 2 concerns linear fractional transformations. This theory is important for next sections. In Sec. 3, we discuss the relationship between linear canonical maps and generating functions. It shows the outline of our idea. Sec. 4 is the continuation and deepening of section 3. It gives the relationship between nonlinear canonical maps and generating functions. In Sec. 5, we give the general Hamilton Jacobi theory. With the aid of the theory, generating functions can be represented as power series in t. It makes the preparation for constructing canonical difference schemes. In Sec. 6, it shows the general method for the construction of canonical difference schemes. Many canonical difference schemes, such as Euler centered scheme, 4–th order centered scheme, staggered explicit scheme and others are presented.

We shall limit ourselves to the local case throughout the paper. Moreover, in this paper we use the older terminologies such as canonicity, canonical maps, etc., in stead of the modern ones such as symplecticity, symplectic maps, etc. So the *canonical* difference schemes can also be called synonymously or even more preferably *symplectic* difference schemes.

§1. Preliminary Facts about Symplectic Geometry

We now review some notions and facts of symplectic geometry [2],[3],[4].

Let $\mathbf{R}^{2n}$ be a $2n$-dim real linear space. The elements of $\mathbf{R}^{2n}$ are $2n$-dim column vectors $z = (z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})^T = (p_1, \cdots, p_n, q_1, \cdots, q_n)^T$. The superscript T represents the matrix transpose.