HAMILTONIAN ALGORITHMS FOR HAMILTONIAN DYNAMICAL SYSTEMS ①②

哈密尔顿动力系统的哈密尔顿算法

§1 Background and Motivation

It is well known that two great contributions in natural science are given by Newton in the 17th century, one being the fundamental law of motion $F = Ma$ in physics, the other being the invention of differential calculus in mathematics. For the motion with n-degree freedom, let

$$\text{vector of position } q = (q_1, \ldots, q_n),$$

$$\text{vector of velocity } \dot{q} = \frac{dq}{dt}(q_1, \ldots, q_n),$$

$$\text{vector of acceleration } \ddot{q} = \frac{d^2}{dt^2}(q_1, \ldots, q_n),$$

force field in conservative mechanical systems be represented by

$$\text{force (vector) } F = -\frac{\partial V}{\partial q},$$

which is the negative gradient of a potential function $V = V(q)$. Then,

$$M\frac{d^2 q}{dt^2} = -\frac{\partial V}{\partial q}. \tag{1.1}$$

This is a standard form of equation of motion and is a system of second order differential equations in the configuration space R^n, usually called the standard form (or Newton's form) in classical mechanics.

In the 18th century Euler and Lagrange introduced the action function

$$L = T - V = \text{kinetic energy} - \text{potential energy}$$

to be the difference between the kinetic and potential energies, i.e.

$$L(q, \dot{q}) = T(\dot{q}) - V(q) = \frac{1}{2}(\dot{q}, M\dot{q}) - V(q).$$

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They show that the actual trajectory is an extremal of the functional on the space of trajectories joining the initial position $q(t_0)$ and final position $q(t_1)$, i.e.

$$\delta \int_{t_0}^{t_1} L(q, \dot{q}) dt = 0. \tag{1.2}$$

In fact, this extremal equation of variational principle (Euler-Lagrange equation)

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0 \tag{1.2'}$$

is equivalent to Newton's equation (1.1). Eq. (1.2) is called Lagrange variational form for classical mechanics.

In the 19th century Hamilton proposed another form by using momentum $p = Mq$ instead of velocity. Then, $T = \frac{1}{2}(p, M^{-1}q)$, total energy $H = T + V$ is represented by a function of p and q, namely,

$$H(p, q) = T(p) + V(q) = \frac{1}{2}(p, M^{-1}p) + V(q),$$

and furthermore,

$$\begin{cases} \dot{p} = -\dfrac{\partial H}{\partial q}, \\ \dot{q} = \dfrac{\partial H}{\partial p}, \end{cases} \tag{1.3}$$

which is called the Hamiltonian system in canonical form. It is seen that (1.3) is a first order differential equation system with variable $(p_1, \ldots, p_n, q_1, \ldots, q_n)$ in $2n$-dimensional phase space or symplectic space and it is in a form with remarkable simplicity and symmetry property. Outline of these three basic forms of equations for classical mechanics can be found in almost all textbooks of theoretical physics and theoretical mechanics. These different mathematical forms describe the same physical law. They are equivalent, but look very different and therefore give different technical approaches in practical "problem solving". So equivalent mathematical formalisms do not imply equal effectiveness in practice. Concerning this we have our understanding throughout our own experience.

In the early 1960s the first author of this paper developed the finite element method — a systematical algorithm for solving stationary problems. This kind of physical problem has two equivalent mathematical formulations: one is Newtonian form, i.e. solving elliptic equation of second order; the other is variational form, i.e. solving extremal of energy functional. The key to success of the finite element method is that variational forms are used as its foundation. After working out the finite element method and its mathematical foundation, the author had tried to apply the idea of this method to dynamical problems of continuum mechanics and failed.

Thus, Lagrange formalism seems not to be the best choice of basis for the numerical methods on nonstationary problem, let alone the Newtonian formalism. So, a more judicious choice might be the Hamiltonian formalism. This inspired our interest towards the Hamiltonian formalism. We also considered the historical inception to Hamiltonian system. Hamilton first originated a mathematical formalism for the foundation of geometrical optics in the 1820's and several years later he applied it to a quite different field, classical mechanics, as an alternative and mathematical equivalent of the then well-founded Newtonian and Lagrangian formalisms. Hamilton had moderate expectations about his own contributions for still wider applications and for a possible formation of a new discipline[1]. However, the acceptance of the Hamiltonian formalism had been slow and sceptical; it was considered generally "beautiful but useless"[2]. Klein, a famous mathematician, while giving a high appreciation to the mathematical elegance of the theory, but suspected its applicability, and said: "Physicists can make use of these theories only very little, and engineers nothing at all"[3]. This "non-Kleinian" remark of Klein was refuted definitively, at least so far as physicists are concerned, by the founding of quantum mechanics, whose formalism is Hamiltonian. Schrödinger, one of the founders of quantum mechanics, has said, "Hamiltonian principle has become the cornerstone of modern physics, $\cdots$. If you wish to apply the modern theory to any particular problem, you must start with putting in Hamiltonian form."[4]

§2 The Significance of Hamiltonian Systems

It is by now almost beyond dispute that, all real physical processes with negligible dissipation — no matter whether it is classical, quantum, or relativistic, and of finite or infinite degrees of freedom — can always be cast in suitable Hamiltonian form.

Finite degrees of freedom. Such as celestial and satellite mechanics, rigid bodies and rigid multi-bodies — including robotic motions, geometrical optics, plasma confinement, accelerator design, optimal control, WKB and ray asymptotics, etc.

Infinite degrees of freedom. Such as ideal fluid dynamics, elasticity, electrodynamics, nonlinear waves, solitons, quantum mechanics and quantum field theory, relativity, etc.

From above, we can see that Hamiltonian system is ubiquitous and it can express different laws of physics in a unified mathematical form. So, a systematic research and development of numerical methodology for Hamiltonian systems is well motivated. If it could turn out to be successful, it would imply wide-ranging applications.

Then is started a search for the existing literature on the numerical methods for Hamiltonian systems. Hamiltonian systems, in finite or infinite dimensions are special forms of ordinary or partial differential equations. From the 18th century up to date, there has existed cumulative wealth of literature on numerical methods for differential equations, no matter whether the methods are in general use or for special problems. However, we were surprised by the puzzling fact that, the pertinent works related specifically to Hamiltonian differential equations are virtually, if not absolutely, void. This gives us added incentive to make an inquiry into this grossly neglected but fertile and promising field.

§3 The Approach Based on Symplectic Geometry

We have illustrated the background, the motivation and the significance of the research. In the following, we shall discuss the scientific approach adopted.

A basic but unwritten rule for the research on numerical methods is that the properties of the original problem should be preserved as much as possible under discretization. The best way to achieve this aim is to work out the analog within the same framework of the original. For example, finite element method is such a method that discrete problems are kept in the same Soblev space consisting of the solutions of the original problem such that some essential properties such as symmetry, positive definite property, conservation law are preserved, guaranteeing the effectiveness and the reliability in practical performance. Some numerical methods which are not so successful provide us with contrary examples to support this rule.

According to the above guideline, numerical methods for Hamiltonian systems which preserve the essential properties of the system are proposed. We called them Hamiltonian algorithms, which can be worked out in the same framework of Hamiltonian systems. In the following, we shall show that symplectic geometry is the mathematical framework of Hamiltonian system. So, Hamiltonian algorithm should be originated from within the framework of symplectic geometry. This is our basic approach for research.

We illustrate concisely symplectic geometry by analogy with Euclidean geometry. An Euclidean structure in Euclidean space R^n is determined by a bilinear, symmetric and nondegenerate inner product

$$\langle x, y\rangle = \langle x, Iy\rangle,\ I = I_n \text{ is identity }. \tag{3.1}$$

When $x \neq 0$, $\langle x, x\rangle$ is positive, and so, we can define the length $\|x\| = \sqrt{\langle x, x\rangle} > 0$. Linear operators which keep inner product (i.e. length) or satisfy $A'A = I$ form a group $O(N)$, i.e. orthogonal group. It is a classical Lie group and its Lie algebra $o(n)$ consists of anti-symmetric operators, i.e. $A' + A = A'I + IA = 0$, or of infinitesimal orthogonal operators.

Symplectic geometry is the geometry of phase space; a symplectic structure in symplectic space, i.e. phase space R^{2n} is determined by a bilinear, anti-symmetric and non-degenerate inner product–symplectic inner product:

$$[x, y] = \langle x, Jy\rangle,\ J = J_{2n} = \begin{pmatrix} 0 & +I_n \\ -I_n & 0 \end{pmatrix}. \tag{3.2}$$

When $n = 1$,

$$[x, y] = \begin{vmatrix} x_1 & y_1 \\ x_2 & y_2 \end{vmatrix}, \tag{3.3}$$

which is the area of the parallelogram formed by vectors x, y. In general, symplectic inner product is area measure. Since symplectic inner product is anti-symmetric, $[x, x] = 0$ for any x, and so it is impossible to define length by symplectic structure. This distinguishes symplectic geometry from Euclidean geometry. Linear operator which keep symplectic inner product, i.e. $A'JA = J$, form a group $Sp(2n)$, i.e. symplectic group. It is also a classical Lie group, and its Lie algebra consists of infinitesimal symplectic operators B, satisfying $B'J + JB = 0$, which is denoted by $sp(2n)$. In odd dimensions anti-symmetric matrix always degenerates, and thus, the dimensions of symplectic space should be even, so should the dimensions of phase space.

In symplectic geometry, a symplectic operator (or, in classical language, canonical transformation) is a diffeomorphism g of R^{2n} onto itself with Jacobi matrix g_z everywhere symplectic. Naturally, this transformation plays an important role in symplectic geometry. Let us come back to the Hamiltonian dynamics. If a pair of n-dimensional vectors are presented as a $2n$-dimensional vector $z = (p, q)$, then canonical Hamiltonian Eq. (1.3) can be written as

$$\frac{dz}{dt} = J^{-1}\nabla H(z), \tag{3.4}$$

and symplectic transformation keeps the canonical form Hamiltonian Eq. (3.4). The fundamental theorem on Hamiltonian formalism says that the solution $z(t)$ of the canonical system (3.4) of energy H with initial value $z(t_0)$ can be generated by a one-parameter group $g^{t,t_0} = g_H^{t,t_0}$, called the phase flow of H, of symplectic operators of R^{2n} (locally in t) such that

$$z(t) = g_H^{t,t_0} z(0),$$

i.e. g_H^{t,t_0} transforms the state at time t_0 to the state at time t. Therefore the evolutions of Hamiltonian dynamical systems are exclusively canonical transformations. This is the fundamental property of Hamiltonian formalism. When the system H is time-independent, then $g_H^{t,t_0} = g_H^{t-t_0,0}$, i.e. the phase flow depends only on the difference of parameters $t - t_0$. For simplicity, we denote it by $g^t = g_H^{t,0}$.

§4 Main Results

Next, we give a brief survey of results of the authors and their colleagues[5,15].

Every difference scheme, explicit or implicit can be regarded as a mapping from time t^n to time t^{n+1}. If the mapping is symplectic we call the difference scheme symplectic scheme.

For example, we consider the linear Hamiltonian system i.e. $H(z) = \frac{1}{2}z'Sz,\ S' = S$. Then, Eq. (3.4) becomes

$$\frac{dz}{dt} = J^{-1}Sz = Lz, \quad L = J^{-1}S.$$

It is easy to see that the weighted Euler scheme

$$\frac{1}{2}(z^{k+1} - z^k) = L(\alpha z^{k+1} + (1-\alpha)z^k) \tag{4.1}$$

for the linear system is symplectic iff $\alpha = \frac{1}{2}$, i.e. it is a time-centered Euler scheme with transition matrix F_τ:

$$z^{k+1} = F_\tau z^k, \quad F_\tau = \varphi(\tau L), \quad \varphi(\lambda) = \frac{1+\lambda/2}{1-\lambda/2}, \tag{4.2}$$

where F_τ, as the Cayley transform of infinitesimally symplectic τL, is symplectic.

For the separable Hamiltonian

$$H(z) = H(p,q) = \frac{1}{2}p'Up + \frac{1}{2}q'Vq \quad (U, V \text{are symmetric matrices}), \tag{4.3}$$

we have Hamiltonian system

$$\begin{aligned} \frac{dp}{dt} &= -Vq, \\ \frac{dq}{dt} &= Up. \end{aligned} \tag{4.4}$$

An explicit scheme

$$\begin{aligned} p^{k+1} &= p^k - \tau V q^k, \\ q^{k+1} &= q^k + \tau U p^{k+1} \end{aligned} \qquad k \geq 0 \tag{4.5}$$

can be rewritten in the form

$$\begin{pmatrix} q^{k+1} \\ p^{k+1} \end{pmatrix} = \begin{pmatrix} I & -\tau V \\ \tau U & I - \tau^2 UV \end{pmatrix} \begin{pmatrix} q^k \\ q^k \end{pmatrix} = g^k \begin{pmatrix} p^k \\ q^k \end{pmatrix}, \tag{4.6}$$

and

$$g^k = \begin{pmatrix} I & -\tau V \\ \tau U & I - \tau^2 UV \end{pmatrix} = \begin{pmatrix} I & 0 \\ -\tau U & I \end{pmatrix} \begin{pmatrix} I - \tau V \\ 0I \end{pmatrix}. \tag{4.7}$$

g^k is symplectic matrix because the right side in Eq. (4.7) is product of two symplectic matrices.

We consider the diagonal Padé approximants $P_m(\lambda)/P_{-m}(\lambda)$ to the exponential function e^{λ}, where

$$
\begin{aligned}
&P_0(\lambda) = 1, \\
&P_1(\lambda) = 2 + \lambda, \\
&P_2(\lambda) = 12 + 6\lambda + \lambda^2, \\
&\quad \ldots, \\
&P_m(\lambda) = 2(2m-1)P_{m-1}(\lambda) + \lambda^2 P_{m-2}(\lambda).
\end{aligned}
$$

We can prove by using generalized Cayley transformation that the difference scheme,

$$z^{k+1} = \frac{P_m(\tau L)}{P_m(-\tau L)} z^k, \quad m = 1, 2, \ldots, \tag{4.8}$$

is symplectic, A-stable, of $2m$th order of accuracy, and of the same set of quadratic invariant integrals including $H(z)$ as that of system (4.9)

$$\frac{dz}{dt} = Lz. \tag{4.9}$$

For the general non-linear Hamiltonian system (3.4), the time-centered Euler scheme

$$z^{k+1} = z^k + \tau J^{-1} H_z\left(\frac{z^{k+1} + z^k}{2}\right) \tag{4.10}$$

is symplectic too, but the trapezoid scheme

$$z^{k+1} = z^k + \tau J^{-1}(H_z(z^{k+1}) + H_z(z^k))/2 \tag{4.11}$$

is not symplectic.

For the nonlinear case of the separable Hamiltonian $H(p,q) = U(p) + V(q)$, like scheme (4.5), the scheme

$$
\begin{aligned}
p^{k+1} &= p^k - \tau V_g(q^k), \\
q^{k+1} &= q^k + \tau U_p(p^{k+1})
\end{aligned} \tag{4.12}
$$

is symplectic. In order to increase the order of accuracy we propose time staggered explicit difference scheme

$$
\begin{aligned}
p^{k+1} &= p^k - \tau V_q(q^{k+\frac{1}{2}}), \\
q^{k+1+\frac{1}{2}} &= q^{k+\frac{1}{2}} + \tau U_p(p^{k+1}).
\end{aligned} \tag{4.13}
$$

Next we consider construction of canonical difference schemes via generating functions. Let

$$\alpha = \begin{bmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{bmatrix}, \quad \alpha^{-1} = \begin{bmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{bmatrix}, \tag{4.14}$$

and α be a non-singular real matrix of order $4n$ satisfying

$$\alpha^T \begin{bmatrix} 0 & I_{2n} \\ I_{2n} & 0 \end{bmatrix} \alpha = \mu \begin{bmatrix} -I_{2n} & 0 \\ 0 & I_{2n} \end{bmatrix}, \quad \text{for some } \mu \neq 0. \tag{4.15}$$

α defines a linear Darboux transformation in product space $R^{2n} \times R^{2n}$ by

$$\begin{bmatrix} \hat{w} \\ w \end{bmatrix} = \alpha \begin{bmatrix} \hat{z} \\ z \end{bmatrix}, \quad \begin{bmatrix} \hat{z} \\ z \end{bmatrix} = \alpha^{-1} \begin{bmatrix} \hat{w} \\ w \end{bmatrix}, \tag{4.16}$$

namely,

$$\begin{aligned} \hat{w} &= A_\alpha \hat{z} + B_\alpha z, \\ w &= C_\alpha \hat{z} + D_\alpha z, \end{aligned} \qquad \hat{z}, z, \hat{w}, w \in R^{2n}. \tag{4.17}$$

Let $z \to \hat{z} = g(z,t) = G(z,t)M_0$, $G(z,t)$ be a phase flow of Hamiltonian system. It is a time-dependent canonical transformation.

The Jacobian

$$M(z,t) = \frac{\partial g(z,t)}{\partial z} \in Sp(2n), \quad M(z,0) = M_0.$$

If

$$\det \mid C_\alpha M_0 + D_\alpha \mid \neq 0 \tag{4.18}$$

holds, then there exists, for sufficiently small $\mid t \mid$ and in (some neighborhood of) R^{2n}, a time-dependent gradient transformation $w \to \hat{w} = f(w,t)$ with Jacobian $\frac{\partial f(w,t)}{\partial w} = N(w,t) \in Sm(2n)$ (i.e. everywhere symmetric), and a time-dependent generating function $\Phi_{\alpha,H}(w,t)$ with gradient

$$f(w,t) = \nabla \Phi_{\alpha,H},$$

$$[w - \nabla \Phi_{\alpha,H}(w,t)] \mid_{\hat{w}=A_\alpha \hat{z}+B_\alpha z, w=C_\alpha \hat{z}+D_\alpha z} = 0$$

is an implicit representation of the canonical transformation $\hat{z} = g(z,t)$. The generating function $\Phi(w,t)$ satisfies the Hamilton-Jacobi equation

$$\Phi_t(w,t) = -\mu H(C_1 \Phi_\alpha(w,t) + D_1 w), \; w = C_\alpha \hat{z} + D_\alpha z. \tag{4.19}$$

On the other hand, for a given time-dependent scalar function $\psi(w,t) : R^{2n} \times R \to R$, we can get a time-dependent canonical map $\tilde{g}(z,t)$. If $\psi(w,t)$ approximates the generating function $\Phi_{\alpha,H}(w,t)$ of the Hamiltonian system (3.1), then $\tilde{g}(z,t)$ approximates the phase flow $g(z,t)$.

For sufficiently small $\tau > 0$ as the time-step, define

$$\psi^{(m)}(w,\tau) = \sum_{k=0}^{m} \Phi^{(k)}(w) \tau^k, \tag{4.20}$$

where

$$\Phi^{(0)}(w) = \frac{1}{2} w^T N_0 w, \; N_0 = (A_\alpha M_0 + B_\alpha)(C_\alpha M_0 + D_\alpha)^{-1},$$

$$\Phi^{(1)}(w) = -\mu H(E_0 w), \; E_0 = (C_\alpha M_0 + D_\alpha)^{-1},$$

and as $k \geq 1$,

$$\Phi^{k+1}(w) = -\frac{\mu}{k+1} \sum_{m=1}^{k} \frac{1}{m!} D_z^m H(E_0 w) \sum_{k_1 + \cdots + k_m = k} (A^\alpha \nabla \Phi^{k_1}(w), \ldots, A^\alpha \nabla \Phi^{k_m}(w)).$$

Then $\psi^{(m)}(w,r)$ is the mth approximant of $\Phi(w,\tau)$, and the gradient map

$$w \to \hat{w} = f(w,\tau) = \nabla \psi^{(m)}(w,\tau) \tag{4.21}$$

defines an implicit canonical map $z \to \hat{z} = g(w,t)$ by the equation

$$[\hat{w} - \nabla \psi_{\alpha,H}(w,t)] \mid_{\hat{w}=A_\alpha \hat{z}+B_\alpha z, w=C_\alpha \hat{z}+D_\alpha z} = 0, \tag{4.22}$$

i.e.

$$A_\alpha \hat{z} + B_\alpha z = \nabla \psi^{(m)}(C_\alpha \hat{z}^{k+1} + D_\alpha z^k, \tau). \tag{4.23}$$

Choose

$$\alpha = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{bmatrix}, \quad \mu = 1, M_0 = J_{2n}.$$

We get generating function of the 1st type for the case $\left|\frac{\partial \hat{q}}{\partial p}\right| \neq 0$:

$$\Phi = \Phi(\hat{q}, q, t,), \quad -\hat{p} = \Phi_{\hat{q}}, \quad p = \Phi_q.$$

Its Hamiltonian-Jacobi equation is

$$\Phi_t + H(\Phi_q, q) = 0.$$

Choose

$$\alpha = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{bmatrix}, \quad \mu = 1, \ M_0 = J_{2n}.$$

We get generating function of the 2nd type for the case $\left|\frac{\partial \hat{q}}{\partial p}\right| \neq 0$:

$$\Phi = \Phi(p, \hat{q}, t,), \quad -\hat{p} = \Phi_{\hat{q}}, \quad -q = \Phi_p, \quad \Phi_t + H(p, -\Phi_p) = 0.$$

Choose Poincare generating transformation

$$\alpha = \begin{bmatrix} -J_{2n} & J_{2n} \\ \frac{1}{2}J_{2n} & \frac{1}{2}J_{2n} \end{bmatrix}, \ \mu = -1, \ M_0 = I_{2n}.$$

We obtain Poincare generating function

$$\Phi = \Phi(w, t), \quad w = \frac{1}{2}(\hat{z} + z), \quad \hat{w} = J(z - \hat{z}) = \Phi_w,$$

$$\Phi_t - H(w - \frac{1}{2}J\Phi_w) = 0.$$

For the linear Darboux transformation α satisfying conditions $A_\alpha + B_\alpha = 0$, $C_\alpha + D_\alpha = I_{2n}$, it can be represented in the following general form

$$\alpha = \begin{vmatrix} -J & J \\ \frac{1}{2}(I+V) & \frac{1}{2}(I-V) \end{vmatrix}, \tag{4.24}$$

where $V^T J + JV = 0$. Therefore, we can construct an infinite variety of symplectic difference schemes via this method.

We now take

$$V = \begin{vmatrix} (1-2\theta)I_n & 0 \\ 0 & -(1-2\theta)I_n \end{vmatrix}. \tag{4.25}$$

It can be easily verified that $V^T J + JV = 0$. When $\theta = 1/2$, the scheme is centered scheme ($V = 0$), which preserves all quadratic first integrals of the Hamiltonian system (1.3). When $\theta \neq 1/2$, the symplectic difference schemes constructed by (4.25) preserve only the quadratic first integrals with the form $\frac{1}{2}z^T \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix} z = p^T B q$ of the Hamiltonian system[17].

A generalization of the above theory and method to the infinite dimensional Hamiltonian equations is also given. Suppose B is a reflexive Banach space and B^* its dual. E^n is an

Euclidean space and n is dimension. The generalized coordinate in the Banach space is function $q(r,t): E^n \times R \to R$. We have $q(r,t) \in B$, which corresponds to the configuration space. We introduce $p(r,t)$, generalized momentum, where $r \in E^n$, $t \in R$. For $\forall t \in T$, $p(r,t) \in B^*$, which corresponds to momentum space, and $B \times B^*$ is the phase space.

Let H be a functional in Hamiltonian mechanics. We have the Hamiltonian equation in $B \times B^*$

$$\begin{aligned} \frac{dq}{dt} &= -\frac{\delta H(p,q,t)}{\delta q}, \\ \frac{dq}{dt} &= +\frac{\delta H(p,q,t)}{\delta p}, \end{aligned} \tag{4.26}$$

where $\delta/\delta q$, $\delta/\delta p$ are variational derivatives. We denote $z=(p,q) \in B \times B^*$. Then we get formally the form of (4.26)

$$\frac{dz}{dt} = J^{-1}\left(\frac{\delta H}{\delta z}\right). \tag{4.27}$$

We cite references on further results of Hamiltonian algorithms, including symmetry and conservation law[9,15,25,27], symplectic Runge-Kutta method[24], multi-stage symplectic schemes[19], leap-frog scheme[21,15], schemes which preserve energy, explicit symplectic schemes and its applications in the Arnold diffusion, chaos computation by symplectic schemes[13], Poisson transformation and its generating function theory and its application[16], applications in quantum mechanics[25], etc.

§5 Conclusion

Our experiences and achievements show that:

1. The numerical methods on Hamiltonian systems is a fertile and promising field and it is worthy of study.

2. Hamiltonian (symplectic) algorithm for Hamiltonian systems can be worked out and would be of great significance. Apart from some rare exceptions, almost all the conventional schemes for ODE's are non-symplectic when applied to Hamiltonian systems. Unavoidably they introduce, above all, artificial dissipation and other parasitic effects which are alien to Hamiltonian dynamics, leading eventually to grave, qualitative distortions. Many nonconventional schemes are proposed, and these schemes have the advantage of preserving the properties of the systems, especially in the aspects of global, structural properties, stability and long-term tracking capabilities, as confirmed by extensive numerical experimentation[9,13].

3. This judiciously chosen symplectic approach is quite natural and justified in view of the innate relationships between Hamiltonian dynamics and symplectic geometry, and the approach turns out to be fruitful and successful. The algorithms are constructed and analysed within the framework of symplectic geometry. For constructing algorithms, we developed the generating function theory in the context of Darboux transformation, which itself is a matter of independent significance.

4. We have also begun to study the Hamiltonian algorithms for quantum mechanics[25]. Hamiltonian algorithms for infinite dimensional Hamiltonian systems–including quantum mechanics and other continuum medium physics–are of promising in applications.

5. Hamiltonian algorithms are also available to dissipative systems. By doubling the variable, we extended dissipative systems as Hamiltonian systems and obtained Hamiltonian

algorithms for them[20,28]. On the other hand, Hamiltonian algorithms can be directly and naturally adapted to Hamiltonian systems with dissipative perturbation given by Rayleigh function. Studies in this field are just beginning and which are also of extensive promise.

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