THE HAMILTONIAN WAY FOR COMPUTING HAMILTONIAN DYNAMICS①

计算哈密尔顿动力学的哈密尔顿方法

Abstract

We present a survey of a recent comprehensive study on the numerical methods for Hamiltonian systems based on symplectic geometry, together the motivations for the research, justification for the symplectic approach adopted, some of the main results, their ramifications and their implications [1-9].

§1 Backgrounds and Motivations

Hamilton originated a mathematical formalism for the foundation of geometrical optics in 1820's and several years later he applied it to a quite different field, i.e., classical mechanics, as an alternative and mathematically equivalent formalism to the then well-founded Newtonian and Lagrangian ones. Hamilton had moderate expectations about his own contributions for still wider applications and for a possible formation of a new discipline [10]. However, the acceptance of Hamiltonian formalism had been slow and sceptical; it was considered generally as "beautiful but useless" [11]. This attitude was best summarized by Klein's recognition of the mathematical elegance of the theory but with an additional remark of caution: "Physicists can make use of these theories only very little, and engineers nothing at all" [12].

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. It is by now almost beyond dispute that, all real physical processes with negligible dissipation can always be cast in suitable Hamiltonian form; and, as Schroedinger has put it, "Hamiltonian principle has become the cornerstone of modern physics, ... If you wish to apply the modern theory to any particular problem, you must start with putting in Hamiltonian form" [13].

At present, Hamiltonian formalism lay at the basis of many diverse fields of physical and engineering sciences such as classical mechanics, satellite orbits, rigid bodies and robotic motions, geometrical optics, plasma confinement, accelerator design, optimal control, WKB and ray asymptotics, fluid dynamics, elasticity, electrodynamics, non-linear waves, solitons, quantum mechanics, relativity, etc. So, a systematic research and development of numerical

①In Spigler R, ed. Applied and Industrial Mathematics. the Netherlands: Kluwer Academic Publisher. 1991: 17–35

methodology for Hamiltonian systems is well motivated. If it turns out to be successful, it would imply wide-ranging applications and give additional evidences for the refutation of Klein's remark by showing that Hamiltonian formalism is not only beautiful but also useful, and, not only useful for theoretical analysis but also useful for practical computations.

After a search into the cumulated wealth of existing literature on numerical methods for differential equations, 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.

§2 The Symplectic Approach

After the initiation of Hamilton, developed further by Jacobi, the most significant progress of the formalism was its geometrization, started since Poincare, resulted in so-called *symplectic geometry*, a new discipline as anticipated by Hamilton, which has become the natural language for Hamiltonian dynamics. Symplectic geometry has the merit to make the deep-lying and intricate properties of dynamics explicit, transparent and easy to grasp. Hamiltonian systems are simply canonical systems on symplectic manifold, i.e., phase space endowed with symplectic structures, the dynamical evolutions are simply symplectic transformations. see e.g., [14]. The desirable algorithms should preserve as much as possible the relevant symplectic properties of the original system. The best way to achieve this aim is to work out the analog within the same framework of the original. So we conceive, construct, analyze and assess numerical algorithms exclusively from within the framework of symplectic geometry. This judiciously chosen approach, inspired by the author's previous experience with the development of the finite element method for solving elliptic equations, is quite natural and justified in view of the innate relationships between Hamiltonian dynamics and symplectic geometry. The approach turns out to be fruitful and successful, and leads to the effective construction as well as the theoretical understanding of an abundance of what we call *symplectic difference schemes*, or symplectic algorithms, or simply *Hamiltonian algorithms*, since they present the *proper* way, i.e., *the Hamiltonian way* for computing *Hamiltonian dynamics*.

Symplectic geometry was developed, due to historical circumstance, mostly for the purposes of theoretical analysis; it lacks the computational component; for example, there is no such theory as that of symplectic approximations for symplectic operators. So, our program might be considered also as an attempt to fill this blank. Generating functions play a key role in the classical transformation theory in symplectic geometry, but they are rather of limited scope in the present setting. So we worked out an extended theory of generating functions in the context of linear Darboux transformations [2,4,6]. This theory leads to our general methodology for the construction and analysis of symplectic schemes. It seems to have its own independent interest in symplectic geometry too.

§3 Some Preliminaries

In real linear space R^{2n}, the vectors will be represented by column matrices $z = (z_1, \dots, z_{2n})'$, the prime $'$ denotes matrix transpose. The *standard symplectic form* in R^{2n} is given by the anti-symmetric, non-degenerate bilinear form

$$\begin{aligned} \omega(x,y) &= x'Jy, \quad \forall x,y \in R^{2n}, \\ J = J_{2n} &= \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \quad J' = -J = J^{-1}. \end{aligned} \tag{1}$$

The symplectic group $Sp(2n)$ consists of the real *symplectic* matrices S preserving ω, i.e., satisfying $S'JS = J$. The corresponding Lie algebra $sp(2n)$ consists of real *infinitesimally symplectic* matrices L satisfying $L'J + JL = 0$, or equivalently $L = JA$, for some symmetric matrix A. The *symplectic product* for two symmetric matrices A, B is defined as $\{A, B\} = AJB - BJA$. Then the space of real *symmetric* matrices $sm(2n)$, under the symplectic product, forms a Lie algebra which is isomorphic to $sp(2n)$ under the usual commutator bracket.

A diffeomorphism g of R^{2n} onto itself is called a *symplectic* operator (or, in classical language, *canonical* transformation) if its Jacobian matrix g_z is everywhere symplectic. A differential map of R^{2n} into itself is called an *infinitesimally symplectic* operator (or, transformation) if its Jacobian matrix is everywhere infinitesimally symplectic. A differential map f of R^{2n} into itself is called a *symmetric* operator (or, transformation) if its Jacobian matrix is everywhere symmetric; in this case, there exists, at least locally, a real function ϕ of R^{2n}, unique up to an additive constant, such that $f = \nabla\phi$, where $\nabla = (\partial/\partial z_1, \ldots, \partial/\partial z_{2n})'$. The space of smooth real functions forms a Lie algebra (of infinite dimensions) $C^\infty(R^{2n})$ under the *Poisson bracket* defined by

$$\{\phi, \psi\} = (\nabla\phi)'J(\nabla\psi). \tag{2}$$

An operator S is symplectic iff it preserves the Poisson bracket, i.e., $\{\phi \circ S, \psi \circ S\} = \{\phi, \psi\} \circ S$. The totality of quadratic forms $\phi_A(z) = (\frac{1}{2})z'Az$, $A' = A$ forms a Lie subalgebra of $C^\infty(R^{2n})$ under Poisson bracket, which is isomorphic to the Lie algebra $sm(2n)$ under the symplectic product.

Choose a smooth function $H \in C^\infty(R^{2n})$, it defines a *Hamiltonian canonical system*

$$\frac{dz}{dt} = J\nabla H(z) \tag{3}$$

on the symplectic space, i.e., phase space R^{2n}, endowed with the symplectic form $\omega(x,y) = x'Jy$. H is called the *Hamiltonian* or *energy* function defining the system. It is customary to split the $z \in R^{2n}$ into two parts $z = (p, q)$, $p_k = z_k$, $q_k = z_{n+k}$, $k = 1, \cdots, n$. In classical language p, q are called position and momentum vectors conjugate to each other. Then $H(z) = H(p, q)$, and equation (3) can be written as

$$\begin{aligned} \frac{dp}{dt} &= -H_q(p,q) \\ \frac{dq}{dt} &= H_p(p,q) \end{aligned} \tag{4}$$

The *fundamental theorem on Hamiltonian formalism* says that the solution $z(t)$ of the canonical system (3) of energy H with initial value $z(0)$ can be generated by a *one-parameter group* $g^t = g^t_H$, called the *phase flow* of H, of symplectic operators of R^{2n} (locally in t) such that

$$z(t) = g^t_H z(0)$$

The system (3) can be written as

$$\frac{d}{dt}(g_H^t z) = J(\nabla H) \circ g_H^t z, \quad \forall z \in R^{2n}$$

The symplecticity of the phase flow implies the class of *conservation laws of phase area* of even dimensions $2m$, $m = 1, \cdots, n$, for the Hamiltonian system (3), the case $m = n$ is the Liouville's conservation law.

Moreover, the Hamiltonian system possesses another class of *conservation laws* related to the *energy* $H(z)$. Consider any smooth function $F(z)$ in R^{2n}, then the composite function $F \circ g_H^t(z)$ satisfies the equation

$$\frac{d}{dt}F \circ (g_H^t z) = \{F, H\} \circ g_H^t z$$

$F(z)$ is called an *invariant* function under the system (3) with Hamiltonian H if $F = F \circ g_H^t$ for all t, this is equivalent to the condition $\{F, H\} = 0$. The energy H itself is always an variant function.

§4 Simple Symplectic Difference Schemes

Consider now the difference schemes for Hamiltonian system (3), restricted mainly to the case of single step (i.e., 2-level) schemes. Time t is discretized into $t = 0, \ \pm\tau, \ \pm 2\tau, \cdots$; τ is the step size, $z(k\tau) \approx z^k$. Each 2-level-scheme is characterized by a *transition* operator relating the old and new states by

$$\hat{z} = G^\tau z, \quad z = z^k, \quad \hat{z} = z^{k+1} \tag{5}$$

$G^\tau = G_H^\tau$ depends on τ, H and the mode of discretization. From the standard-point of symplectic geometry, it is natural and even mandatory to require G_H^τ to be symplectic. A difference scheme for Hamiltonian system (3) is called *symplectic* (or, *canonical*) if its transition operator G_H^τ is symplectic for all Hamiltonian functions H and step sizes τ. We shall also consider difference schemes non-symplectic in this general sense, but are symplectic for special classes of Hamiltonians. The true solution relating the old and new states is

$$z((k+1)\tau) = g_H^t z(k\tau),$$

So we are confronted with the problem of symplectic approximation to the symplectic phase flow g_H^τ. For the latter there is a Lie expansion in τ

$$(g_H^\tau z)_i = z_i + \tau\{z_i, H\} + \frac{\tau^2}{2!}\{\{z_i, H\}, H\} + \cdots, \quad i = 1, \cdots, 2n. \tag{6}$$

Although the truncations give "legitimate" approximations, but they are non-symplectic in general, so undesirable.

Consider the simplest one-legged weighted Euler scheme for (3)

$$\hat{z} = z + \tau J(\nabla H)(c\hat{z} + (1-c)z) \tag{7}$$

where c is a real constant. It is easy to show that it is symplectic iff $c = \frac{1}{2}$. The only symplectic case corresponds to the *time-centered Euler scheme*

$$\hat{z} = z + \tau J(\nabla H)(\frac{\hat{z} + z}{2}) \tag{8}$$

This simple proposition illustrate a general situation: apart from some very rare exceptions, the vast majority of conventional schemes are non-symplectic. However, if we allow c in (7) to be a *real matrix of order* $2n$, we get a far-reaching generalization: (7) *is symplectic* iff

$$c = \frac{1}{2}(I_{2n} + J_{2n}B), \quad B' = B \tag{9}$$

The symplectic case corresponds to

$$\hat{z} = z + \tau J(\nabla H)(\frac{1}{2}(I + JB)\hat{z} + \frac{1}{2}(I - JB)z), \quad B' = B, \tag{10}$$

They are all implicit, (10) is solvable for new $\hat{z}$ in terms of old z whenever $|\tau|$ is small enough. (10) enjoy many properties in common with (3), they may be considered as *Hamiltonian difference equations.*

Let the transition in (10) to be

$$z^{k+1} = G^{\tau}_{H,B} z^k, \tag{11}$$

for $B = 0$, the accuracy order is 2, For $B \neq 0$, the order is 1; however, the alternating composite schemes given by

$$z^{k+1} = G^{\tau}_{H,\pm B} z^k, \tag{12}$$

where

$$\begin{aligned} G^{\tau}_{H,\pm B} &= G^{\frac{\tau}{2}}_{H,B} \circ G^{\frac{\tau}{2}}_{H,-B} \\ G^{\tau}_{H,\mp B} &= G^{\frac{\tau}{2}}_{H,-B} \circ G^{\frac{\tau}{2}}_{H,B} \end{aligned} \tag{13}$$

have accuracy order 2.

So we get a great variety of simple symplectic schemes of order 1 or 2, classified according to type matrices $B \in sm(2n)$, which is a linear space of dimension $2n^2 + n$.

The conservation properties of the above symplectic schemes are well-understood. In fact we have proved:

Let $\phi_A(z) = \frac{1}{2}z'Az$, $A' = A$ be a quadratic form and A commutes symplectically with the type matrix B, i.e., $AJB = BJA$. Then ϕ_A is invariant under the system with Hamiltonian H iff ϕ_A is invariant under symplectic difference schemes (10) of types $G^{\tau}_{H,B}$, $G^{\tau}_{H,-B}$.

We list some of the most important types B together with the corresponding form of symplectic matrices A of the conserved quadratic invariants ϕ_A:

$B = 0$, $\quad A$ arbitrary.

$B = \pm\begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix} = \pm E_{2n}$, $\quad A = \begin{pmatrix} 0 & b \\ b' & 0 \end{pmatrix}$, $\quad b$ arbitrary; angular momentum type.

$B = \pm I_{2n}$, $\quad A = \begin{pmatrix} a & b \\ -b & a \end{pmatrix}$, $\quad a' = a$, $b' = -b$; Hermitian type.

$B = \pm\begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix} = \pm I_{n,n}$, $\quad A = \begin{pmatrix} a & b \\ -b & -a \end{pmatrix}$, $\quad a' = a$, $b' = -b$.

§5 Explicit Symplectic Schemes

The symplecticity of Hamiltonian dynamical evolutions implies some kind of symmetry between the past and the future. So symplectic schemes are implicit by nature. However, for special classes of Hamiltonians of practical importance, and for certain type matrices B (see 4), the corresponding simple symplectic schemes will be practically explicit, leading to simple and fast algorithms. For example, consider the "separable" Hamiltonians of the form

$$H(p,q) = \phi(p) + \psi(q), \tag{14}$$

where ϕ, ψ are functions of n variables, then

$$H_p(p,q) = \phi_p(p), \quad H_q(p,q) = \psi_q(q).$$

Most of the energy functions in classical mechanics are separable in the above sense. Apply symplectic schemes (10) of type E_{2n}, and we get explicit schemes

$$\begin{aligned} &\text{Type} \quad E_{2n}; \qquad \hat{p} = p - \tau\psi_q(q), \quad \hat{q} = q + \tau\phi_p(\hat{p}). \\ &\text{Type} \quad -E_{2n}; \quad \hat{p} = p - \tau\psi_q(\hat{q}), \quad \hat{q} = q + \tau\phi_p(p). \end{aligned} \tag{15}$$

The accuracy of this scheme can be raised without additional labor by putting p (or q) at integer times and q (or p) at half-integer times, we get *time-staggered symplectic* scheme of order 2, explicit for separable Hamiltons:

$$p^{k+1} = p^k - \tau\psi_q(q^{k+\frac{1}{2}}), \quad q^{k+1+\frac{1}{2}} = q^{k+\frac{1}{2}} + \tau\phi_p(p^{k+1}). \tag{16}$$

This explicit symplectic scheme was used and explained in detail by Feynman in his Lectures for computing the motions of an oscillating spring and of a planet around the sun [11]. The staggering (in time and/or in space) is a useful numerical technique for improving accuracy and symmetry.

The oldest and simplest among all difference schemes is the explicit Euler method

$$\hat{z} = z + \tau J\nabla H(z) = (I + \tau J\nabla H)(z) = G_H^\tau(z). \tag{17}$$

It is interest to ask: under what conditions on H the operator G_H^τ will be symplectic. We have proved: If, in R^{2n}

$$H(p,q) = \phi(Ap + Bq), \qquad AB' = BA' \tag{18}$$

where ϕ is a function of n variable, A, B are matrices of order n; then G_H^τ is symplectic and exact, i.e., $G_H^\tau = g_H^\tau$.

If, moreover

$$H(p,q) = \sum_{i=1}^{m} H_i(p,q), \quad H_i(p,q) = \phi_i(A_i p + B_i q), \quad A_i B_i' = B_i A_i' \tag{19}$$

Where ϕ_i are functions of n variables, A_i, B_i are matrices of order n. Let $[s_1, s_2, \cdots, s_m]$ be an arbitrary permutation of $[1, 2, \cdots, m]$; then the following scheme is symplectic and of order 1:

$$z \to \hat{z} = (G^\tau[s_1, s_2, \cdots, s_m])z, \quad G^\tau[s_1, s_2, \cdots, s_m] = (G^\tau[s_1]) \circ (G^\tau[s_2]) \circ \cdots \circ (G^\tau[s_m]) \tag{20}$$

where $G^\tau[i] = G_{H_i}^\tau$. Moreover, the following alternating composite is symplectic and of order 2:

$$z \to \hat{z} = (G^{\frac{\tau}{2}}([s_1, s_2, \cdots, s_m]) \circ (G^{\frac{\tau}{2}}[s_m, \cdots, s_2, s_1])z \tag{21}$$

Note that the explicit symplectic schemes of order 1 and 2 of type $\pm E_{2n}$ for separable Hamiltonian in the sense of (14) are special cases of the above situation. We have computed with success using (19-21) the systems with Hamiltonians [18,19]

$$H_k(p,q) = \sum_{j=1}^{k} \cos(p \cos \frac{2\pi j}{k} + q \sin \frac{2\pi j}{k}) \tag{22}$$

with k-fold rotational symmetry in phase plane. They are not separable in the sense of (14) when $k \neq 1, 2, 4$.

For the general characterization for the symplecticity of explicit Euler schemes, we have proved: $G_H^\tau = I + \tau J \nabla H$ in R^{2n} is symplectic iff

$$H_{zz} J H_{zz} = 0, \quad \forall z \in R^{2n} \tag{23}$$

where H_{zz} is the Hessian matrix of H.

Furthermore we have an as yet incomplete but interesting characterization of (23) as follows:

A necessary and sufficient condition for $H_{zz} J H_{zz} \equiv 0$ in R^{2n} is that

$H(z) = H(p,q)$ can be expressed, under suitable *linear symplectic and orthogonal transformation* $z = Sw$, $w = (u,v)$, as

$$H(S(u,v)) = \phi(u) + \psi(v), \quad \psi \text{ is linear}, \quad S \in Sp(2n) \cap O(2n) \tag{24}$$

i.e., separable in sense of (14) with additional linearity in ψ.

The "sufficiency" part follows easily from the propositions stated above. However, the "necessity" part is not yet fully established. We have proved for the case that H is a quadratic form. Moreover for $n = 1$, (23) is equivalent to the Monge-Ampere equation $|H_{zz}| = 0$, so H defines a global surface of zero Gaussian curvature in R^3, the assertion is a consequence of a global theorem on developable surface in R^3 [16,17]. Since the global strong degeneracy condition (23) should imply drastic simplification of the profile of function H, so we have reasons to suggest the conjecture (23) $\Rightarrow$ (24).

§6 Symplectic Schemes for Linear Hamiltonian Systems

By a linear Hamiltonian system here we mean the system with a quadratic form $H(z) = \phi_A(z) = (z'Az)/2, \quad A' = A$ as the Hamiltonian. Then the system becomes

$$\frac{dz}{dt} = J \nabla \phi_A(z) = JAz \tag{25}$$

with phase flow

$$g_H^t = \exp(tJA) = I + \sum_{k=1}^{\infty} \frac{t^k}{k!} (JA)^k \tag{26}$$

as linear symplectic operators. All the constructions of symplectic schemes in Section 4 and in Sections 7 and 8 below can be applied, but here we present the approach of symplectic approximations to the exponential [1,2,9]. The Taylor series in (27) can be arbitrarily truncated, but apart from some rare exceptions, symplectic approximations can not be provided. The natural way is looking for rational and especially the Padé approximations of the exponential function $\exp(\lambda)$.

$$\exp(\lambda) - \frac{P_{m,l}(\lambda)}{Q_{m,l}(\lambda)} = O(|\lambda|^{m+l+1}), \quad |\lambda| \sim 0 \tag{27}$$

$P_{m,l}$ and $Q_{m,l}$ is of degree m, l respectively. It can be proved that, the matrix Padé transform $P_{m,l}(\tau JA)/Q_{m,l}(\tau JA)$ is symplectic iff the Padé approximant is diagonal, i.e., $m = l$; then $P_{m,m}(\lambda) = P_m(\lambda)$, $Q_{m,m}(\lambda) = P_m(-\lambda)$, and

$$\begin{aligned} &P_0(\lambda) = 1, \\ &P_1(\lambda) = 2 + \lambda, \\ &P_2(\lambda) = 12 + 6\lambda + \lambda^2, \\ &P_m(\lambda) = 2(2m-1)P_{m-1}(\lambda) + \lambda^2 P_{m-2}\lambda) \end{aligned} \tag{28}$$

We get the *Padé symplectic* scheme

$$P_m(-\tau JA)\hat{z} = P_m(\tau JA)z, \quad \hat{z} = G^\tau z = \frac{P_m(\tau JA)}{P_m(-\tau JA)}z. \tag{29}$$

which is of order $2m$. For $m = 1$ we get the time-centered Euler scheme (8).

It is known that every linear system (26) in R^{2n} with $H = \phi_A$ is completely integrable in the sense that there exists n invariant quadratic forms, $\phi_{A_1} = \phi_A, \cdots, \phi_{A_n}$ which are functionally independent and mutually commuting $\{\phi_{A_i}, \phi_{A_j}\} = 0, \quad i,j = 1, \cdots, n$. The *Padé symplectic schemes* have the remarkable property that they possess *the same set of invariant quadratic forms* as that of the original linear Hamiltonian system. If the original linear phase flow is not only symplectic but also unitary, then the Padé schemes are also unitary, so they are useful for quantum mechanical applications.

In general, the linear symplectic schemes for linear Hamiltonian system, even when they do not preserve the quadratic invariants (including the energy) of the original system, we still can construct for any linear symplectic transition operator G_H^τ (in fact even for any $G \in Sp(2n)$) a set of n independent, mutually commuting quadratic forms ϕ_{B_i} which are invariant under G. This set is near to the corresponding set of the original when τ is small, so they behave well in the aspects of orbital structure and stability.

§7 Symplectic Leap-frog Schemes

The concept of symplecticity for multi-level schemes for Hamiltonian system is more complicated then the 2-level case . We discuss only the 3-level schemes. For system (3) with Hamiltonian H and phase flow operator g_H^t, we have the following exact relations between the solution at 3 successive moments, we fix $\tau > 0$ and t:

$$z(t) \to z(t+\tau) = g_H^\tau z(t)$$
$$z(t) \to z(t-\tau) = g_H^{-\tau} z(t)$$

Then we have

$$z(t+\tau) - z(t-\tau) = \delta_H^\tau z(t), \quad \delta_H^\tau = g_H^\tau - g_H^{-\tau} \tag{30}$$

where δ_H^τ is the exact difference operator for the Hamiltonian system, and can be shown to be infinitesimally symplectic, i.e., its Jacobian matrix belongs to $sp(2n)$ everywhere.

We take the general form of 3-level leap-frog schemes as

$$z^{k+1} - z^{k-1} = \Delta_H^\tau z^k \tag{31}$$

here the coefficients chosen before z^{k+1} and z^{k-1} are justified on grounds of symmetry. The *leap-frog* scheme (31) is called *symplectic* if the operator Δ_H^τ is *infinitesimally symplectic*. So our problem is to seek for approximations Δ_H^τ to δ_H^τ preserving infinitesimal symplecticity.

For linear Hamiltonian system (25, 26) we have

$$\delta_H^\tau = \exp(\tau JA) - \exp(-\tau JA) = 2\sinh(\tau JA) = 2\sum_{j=1}^{\infty} \frac{(-1)^j}{(2j-1)!}(\tau JA)^{2j-1} \tag{32}$$

here all the truncations are infinitesimally symplectic, so we get symplectic leap-frog schemes

$$\begin{aligned} &\text{order } 2: \quad z^{k+1} - z^{k-1} = 2\tau JAz^k \\ &\text{order } 2m: \quad z^{k+1} - z^{k-1} = 2\Big(\sum_{j=1}^{m} \frac{(-1)^j}{(2j-1)!}(\tau JA)^{2j-1}\Big)z^k. \end{aligned}$$

Similarly, for non-linear Hamiltonian system, from the Lie series (6) of phase flow we get

$$(\delta_H^\tau z)_i = 2\sum_{j=1}^{\infty} \frac{\tau^{2j-1}}{(2j-1)!}\{\{\cdots\{\{z_i^k, H\}, H\}\cdots, H\}, H\} \tag{33}$$

whose truncations provide *symplectic leap-frog* schemes *

$$\text{order } 2: \quad z^{k+1} - z^{k-1} = 2\tau J\nabla H(z^k) \tag{34}$$

$$\text{order } 2m: \quad z_i^{k+1} - z_i^{k-1} = \delta_{H,m}^\tau z^k \tag{35}$$

where $\delta_{H,m}^\tau z$ is the m-term truncation of (33).

For these schemes we can establish the conservation property as: If $F(z) = z'Bz$ is a quadratic invariant under g_H^t, then follows the "cross invariance" under the scheme (34)

$$(z^{k+1})'Bz^k = (z^k)'Bz^{k-1}.$$

All the symplectic leap-frog schemes are explicit. The simplest 2nd order scheme (34) is one of the rare cases of existing methods which are symplectic and seems to be the oldest one. It is interesting to note that, according to linearized analysis, the stability domain for (34) is only a segment on the imaginary axis in the complex plane, it is absolutely unstable when applied to asymptotically stable systems. However, it works well with Hamiltonian systems, which correspond to the critical case with pure imaginary characteristic exponents and are never asymptotically stable owing to the symplecticity of dynamics.

§8 Fractional Transforms and Generating Functions

A matrix α of order $4n$ is called a *Darboux matrix* if

$$\begin{aligned} &\alpha' J_{4n}\alpha = \tilde{J}_{4n} \quad J_{4n} = \begin{pmatrix} 0 & -I_{2n} \\ I_{2n} & 0 \end{pmatrix}, \quad \tilde{J}_{4n} = \begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix}, \\ &\alpha = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \alpha^{-1} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}, \end{aligned} \tag{36}$$

Each Darboux matrix induces a (linear) *fractional transform* between symplectic and symmetric matrices

$$\begin{aligned} &\sigma_\alpha: \quad Sp(2n) \to sm(2n) \\ &\sigma_\alpha(S) = (aS+b)(cS+d)^{-1} = A, \quad \text{for} \quad |cS+d| \neq 0 \end{aligned} \tag{37}$$

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* This is incorrect. They are non-symplectic. The author noticed it and gave the note on his reprint.

with inverse transform $\sigma_\alpha^{-1} = \sigma_{\alpha^{-1}}$

$$\begin{aligned} &\sigma_\alpha^{-1}: \qquad sm(2n) \to Sp(2n), \\ &\sigma_\alpha^{-1}(A) = (a_1 A + b_1)(c_1 A + d_1)^{-1} = S, \quad \text{for} \quad |c_1 A + d_1| \neq 0. \end{aligned} \tag{38}$$

The above machinery can be extended to generally non-linear operators in R^{2n}. Let $Symp(2n)$ denote the totality of symplectic operators, and $symm(2n)$ denote the totality of symmetric operators. Each $f \in symm(2n)$ corresponds, at least locally a real function ϕ (up to a constant) such that $f(w) = \nabla\phi(w)$. Then we have

$$\begin{aligned} &\sigma_\alpha: \qquad Symp(2n) \to symm(2n), \\ &\sigma_\alpha(g) = (ag + b)(cg + d)^{-1} = \nabla\phi, \quad \text{for} \quad |cg_z + d| \neq 0, \end{aligned} \tag{39}$$

or alternatively

$$ag(z) + bz = (\nabla\phi)(cg(z) + dz), \tag{40}$$

where ϕ is called the *generating function* of Darboux type α for the symplectic operator g. Then

$$\begin{aligned} &\sigma_\alpha^{-1}: \qquad symm(2n) \to Symp(2n), \\ &\sigma_\alpha^{-1}(\nabla\phi) = (a_1 \nabla\phi + b_1)(c_1 \nabla\phi + d_1)^{-1} = g, \quad \text{for} \quad |c_1 \phi_{ww} + d_1| \neq 0 \end{aligned} \tag{41}$$

or alternatively

$$a_1 \nabla\phi(w) + b_1(w) = g(c_1 \nabla\phi(w) + d_1 w), \tag{42}$$

where g is called the symplectic operator of Darboux type α for the generating function ϕ.

For the study of symplectic difference algorithms we may narrow down the class of Darboux matrices to the subclass of *normal Darboux matrices*, i.e., those satisfying $a+b=0$, $c+d=I_{2n}$. The normal Darboux matrices α can be characterized as

$$\begin{aligned} \alpha &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} J & -J \\ \frac{1}{2}(I+JB) & \frac{1}{2}(I-JB) \end{pmatrix}, \quad B' = B \\ \alpha^{-1} &= \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(JBJ - J) & I \\ \frac{1}{2}(JBJ + J) & I \end{pmatrix}. \end{aligned} \tag{43}$$

The fractional transform induced by normal Darboux matrix establishes a 1-1 correspondence between *symplectic operators near identity* and *symmetric operators near nullity*. Then the determinantal conditions could be taken for granted. Those B listed in 4 correspond to the most important normal Darboux matrices.

For each Hamiltonian H with its phase flow g_H^t and for each normal Darboux matrix α, we get the *generating function* $\phi = \phi_H^t = \phi_{H,\alpha}^t$ of *normal Darboux type* α for the *phase flow* of H by

$$\nabla\phi_{H,\alpha}^t = (ag_H^t + b)(cg_H^t + d)^{-1}, \quad \text{for small} \quad |t|. \tag{44}$$

$\phi_{H,\alpha}^t$ satisfies the *Hamilton-Jacobi* equation

$$\frac{\partial}{\partial t}\phi = -H(a_1 \nabla\phi(w) + b_1 w) = -H(c_1 \nabla\phi(w) + d_1 w) \tag{45}$$

and can be expressed by Taylor series in t

$$\phi(w,t) = \sum_{k=1}^{\infty} \phi^{(k)}(w) t^k, \quad |t| \quad \text{small}. \tag{46}$$

The coefficients can be determined recursively

$$\phi^{(1)}(w) = -\,H(w), \quad \text{and for} \quad k \geq 0, \quad a_1 = \frac{1}{2}(JBJ - J):$$

$$\phi^{(k+1)}(w) = \frac{-1}{k+1} \sum_{m=1}^{k} \frac{1}{m!} \sum_{i_1,\cdots,i_n=1}^{2n} \sum_{\substack{j_1+\cdots+j_m=k \\ j_l \geq 1}} H_{z_{i_1}\cdots z_{i_m}}(w)$$

$$\times\, (a_1 \nabla \phi^{(j_1)}(w))_{i_1} \cdots (a_1 \nabla \phi^{(j_m)}(w))_{i_m}. \tag{47}$$

Let ψ^τ be a truncation of $\phi^\tau_{H,\alpha}$ up to certain power t^m, say. Using inverse transform σ_α^{-1} we get the symplectic operator

$$G^\tau = \sigma_\alpha^{-1}(\nabla \psi^\tau), \quad |\tau| \quad \text{small}$$

which depends on τ, H, α (or equivalently B) and the mode of truncation. It is a symplectic approximation to the phase flow g_H^τ and can serve as the transition operator of a symplectic difference scheme (for the Hamiltonian system (3))

$$\hat{z} = G^\tau z \tag{48}$$

which, by (39,40,41) can be written as

$$J\hat{z} - Jz = \nabla \psi^\tau(c\hat{z} + (I - c)z), \quad c = \frac{1}{2}(I + JB). \tag{49}$$

Thus, using the machinery of phase flow generating functions we have constructed, for each H and each normal Darboux matrix, an hierarchy of symplectic schemes by truncation. The simple symplectic schemes in 4 corresponds to the lowest truncation. The conservation properties of all these higher order schemes are the same as stated in 4.

§9 Numerical Experiments and Discussions

Numerical experimentation shows strong evidences of superior performance of symplectic schemes over the non-symplectic ones. Most of the conventional schemes 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.

On the other hand, symplectic schemes tend to purify (sometimes even simplify) the algorithms, inhibiting artificial dissipations and all other non-Hamiltonian distortions. We present a comparative study for the harmonic oscillator, Fig 1,2 and for a nonlinear oscillator, Fig 3,4. For some other result, see [4]. The non-symplectic Runge-Kutta scheme yields persistent spiraling of phase trajectories with artificial creation of attractors (impossible for Hamiltonian system), irrespective of the higher order of the scheme and the smallness of step sizes. The symplectic scheme always give clear-cut invariant elliptical trajectories even for low order of schemes and large step sizes. The striking contrast is, at least, in the aspects of global and structural preservation and long-term tracking capabilities.

The most important characteristic property of Hamiltonian dynamics is the intricate *coexistence* of *regular* and *chaotic* motions, as implied by the celebrated KAM theorem [14]. The advantage of symplectic schemes consists primarily in the essential fidelity to the original in this aspect. The behavior of symplectic schemes should be and could be understood and analyzed in the context of KAM theory on preservation and break-down of invariant tori. There are evidences showing that an analog of KAM theorem should hold for symplectic symplectic difference schemes, we have a related result for a simple special case.

Symplectic schemes for Hamiltonian systems do not imply non-Hamiltonian perturbations, but they do inevitably imply Hamiltonian perturbations. An example is the break-down of invariant tori when the scheme is applied to integrable or near integrable systems. The effect is indiscernible for small step size, but becomes pronounced with large step sizes, see Fig 5. Another example is the *artificial chaos* in the form of Arnold diffusion. We computed by explicit symplectic schemes (21) of order 2, the Hamiltonian system H_k (22) with k-fold rotational symmetry in 1 degree of freedom, suggested by Sagdeev, Zaslavsky *et al* [18] in the context of chaotic stream lines of Lagrangian turbulence, see also [19-21]. Fig 6 gives some results for $k = 4$, when initial point is chosen on the original separatrix, the diffusion shows a remarkable combination of *regularity* and *chaoticity*, almost rectilinear motion along the "highways" and random turning at the "crossroads". Fig 7,8 give some results for $k = 3, 5$. For $k = 5$ the orbit is reminiscent of Alhambra fresco decoration or Penrose tiling or quasi-crystal with 10-fold symmetry. It is worth to note the connections of symplectic schemes with these widely different topics.

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Fig.1. Harmonic oscillator $H = (p^2 + a^2 q^2)/2, \quad a = 2.$
Runge-Kutta method, order 4, non-symplectic.
stepsize=τ, total number of steps = N, number of steps per plot = M.
Single orbit is computed in all cases with the same initial point.
Upper-left: $\tau = 0.5$, $N = 2000$, $M = 1$. Upper-right: $\tau = 0.1$, $N = 2000$, $M = 1$.
Lower-left: $\tau = 0.3$, $N = 2000$, $M = 1$. Lower-right: $\tau = 0.1$, $N = 200000$, $M = 100$.

For large stepsize 0.5 (upper-left), the orbit spirials quickly around and towards the origin with a wrong formation of an artificial attractor there. The dissipation effect diminishes with smaller stepsize 0.3 (lower-left), but still pronounced. At very small stepsize 0.1 (upper-right), the orbit appears to be well-behaved as a closed ellipse when total number of steps is limited to 2000 as before. However, the artificial dissipation eventually becomes pronounced again when computed to twenty thousands steps (lower-right).

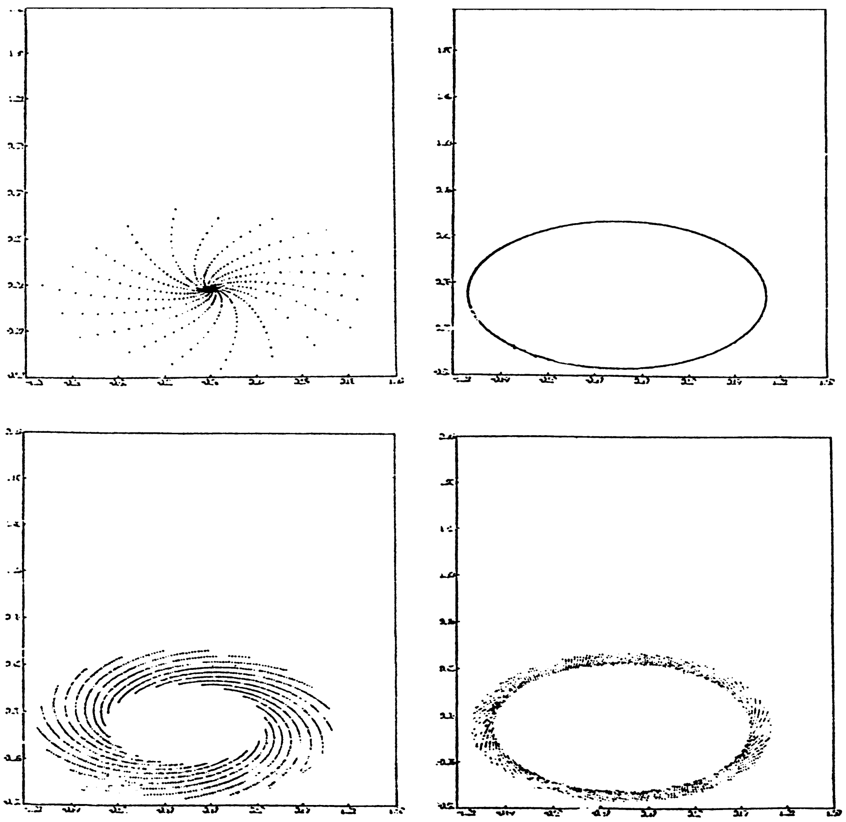


Fig.2. Harmonic oscillator $H = (p^2 + a^2 q^2)/2, \quad a = 2.$

Explicit symplectic composite scheme, order 2

stepsize=τ, total number of steps $= N$, number of steps per plot $= M$.

Single orbit is computed in all cases with the same initial point.

Upper-left: $\tau = 0.5$, $N = 2000$, $M = 1$. Upper-right: $\tau = 0.1$, $N = 2000$, $M = 1$.

Lower-left: $\tau = 0.3$, $N = 2000$, $M = 1$. Lower-right: $\tau = 0.1$, $N = 1000000$, $M = 500$.

The arrangement of calculation is just the same as in Fig.1 for comparison. In all cases the symplectic computing gives always clear-cut invariant ellipses even for the very long run of a million steps (upper-right). The artificial dissipation is fully inhibited. The computational stability and the ability for long time tracking and the preservation of the structure of the phase portrait is truely remarkable. We note that the specific symplectic scheme used here does not preserve the quadratic energy exactly but it does possess an invariant quadratic form whose level lines are ellipses very close to and practically indistinguishable from the original ellipses.

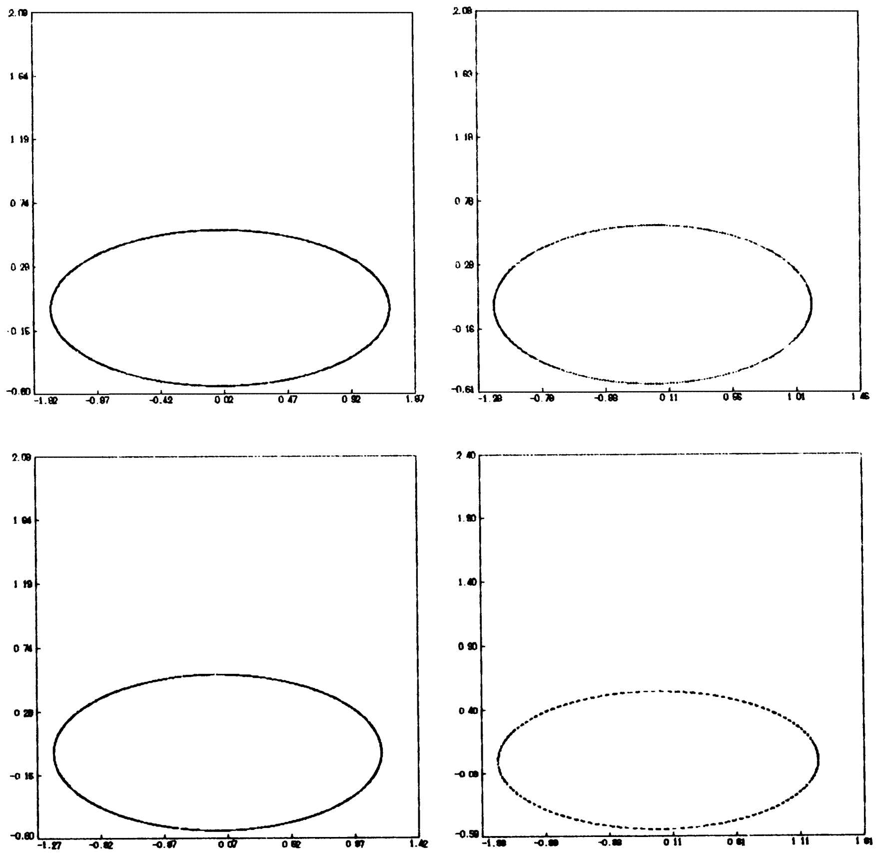


Fig.3. Nonlinear oscillator $H = (p^2 + a^2q^2 + a^4q^4/12)/2, \quad a = 2.$
Runge-Kutta method, order 4, non-symplectic.
stepsize=τ, total number of steps = N, number of steps per plot = M.
Single orbit is computed in all cases with the same initial point.
Upper-left: $\tau = 0.5$, $N = 2000$, $M = 1$. Upper-right: $\tau = 0.1$, $N = 2000$, $M = 1$.
Lower-left: $\tau = 0.3$, $N = 2000$, $M = 1$. Lower-right: $\tau = 0.1$, $N = 200000$, $M = 100$.

This nonlinear oscillator is the harmonic one plus a nonlinear perturbation. At low energy values the invariant orbits are only nearly elliptical in form. For larger stepsizes 0.5 (upper-left), and 0.3 (lower-left), the spiraling structures of the orbits are much more complicated then the corresponding linear cases in the left hand side of Fig.1. At very small stepsize 0.1 (upper-right and lower-right), the situation is again similar to the linear case with the eventual cumulative artificial dissipation noticeable in the long run. Artificial dissipation is inevitable for both linear and nonlinear cases in non-symplectic schemes.

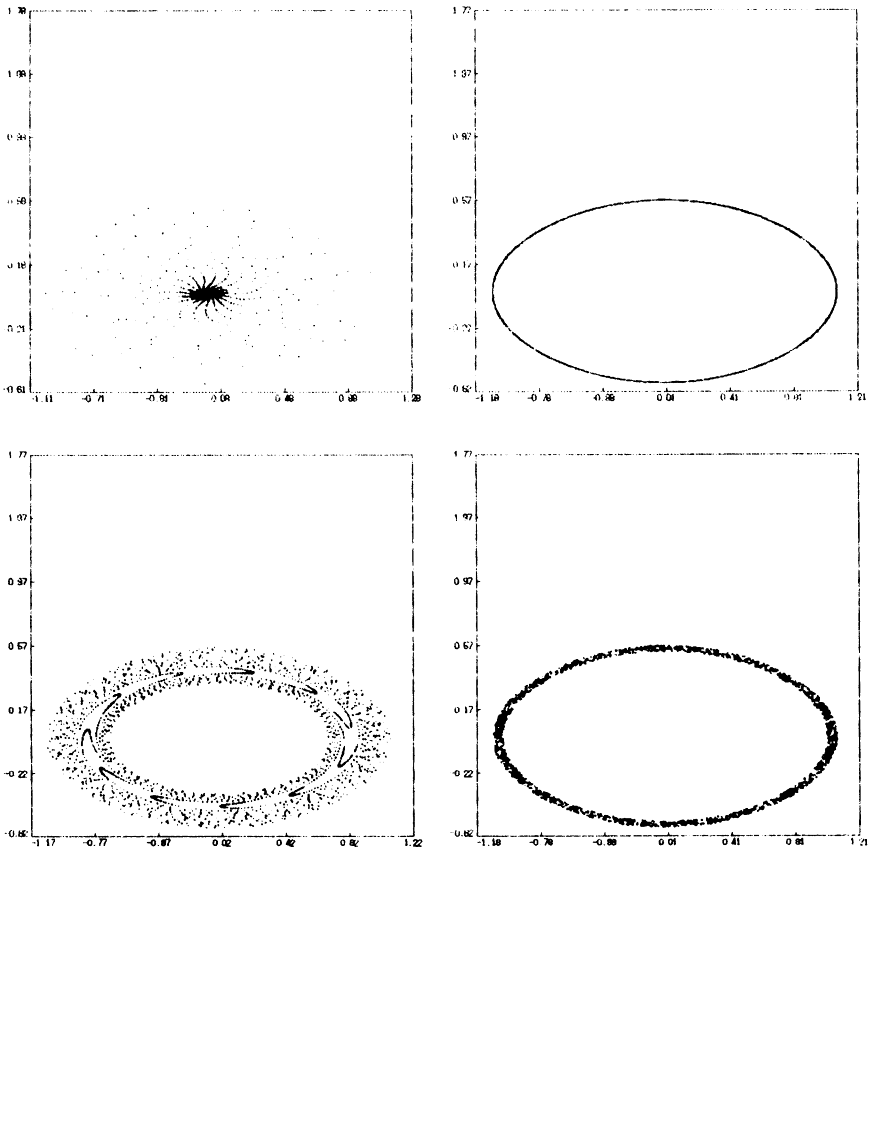


Fig.4. Nonlinear oscillator $H = (p^2 + a^2q^2 + a^4q^4/12)/2, \quad a = 2.$
Explicit symplectic composite scheme, order 2.
stepsize=τ, total number of steps = N, number of steps per plot = M.
Single orbit is computed in all cases with the same initial point.
Upper-left: $\tau = 0.5$, $N = 2000$, $M = 1$. Upper-right: $\tau = 0.1$, $N = 2000$, $M = 1$.
Lower-left: $\tau = 0.3$, $N = 2000$, $M = 1$. Lower-right: $\tau = 0.1$, $N = 1000000$, $M = 500$.

Here again the symplectic computing gives always clear-cut invariant closed orbits including the run of a million steps without any dissipation. The computed orbits are only nearly elliptical but hardly discernible from the ellipses in Fig.2. The apparent identity of all the orbits in Fig.1 and 2 shows the stability and robustness of the method. From Fig.1-4 one sees the sharp contrast between the performances of the two methods. The symplectic method is far superior at least in the aspects of computational stability, global and structural preservation and long-term simulation. Incidentally the specific 2nd order symplectic method adopted is 4 times faster than the 4th order Runge-Kutta method.

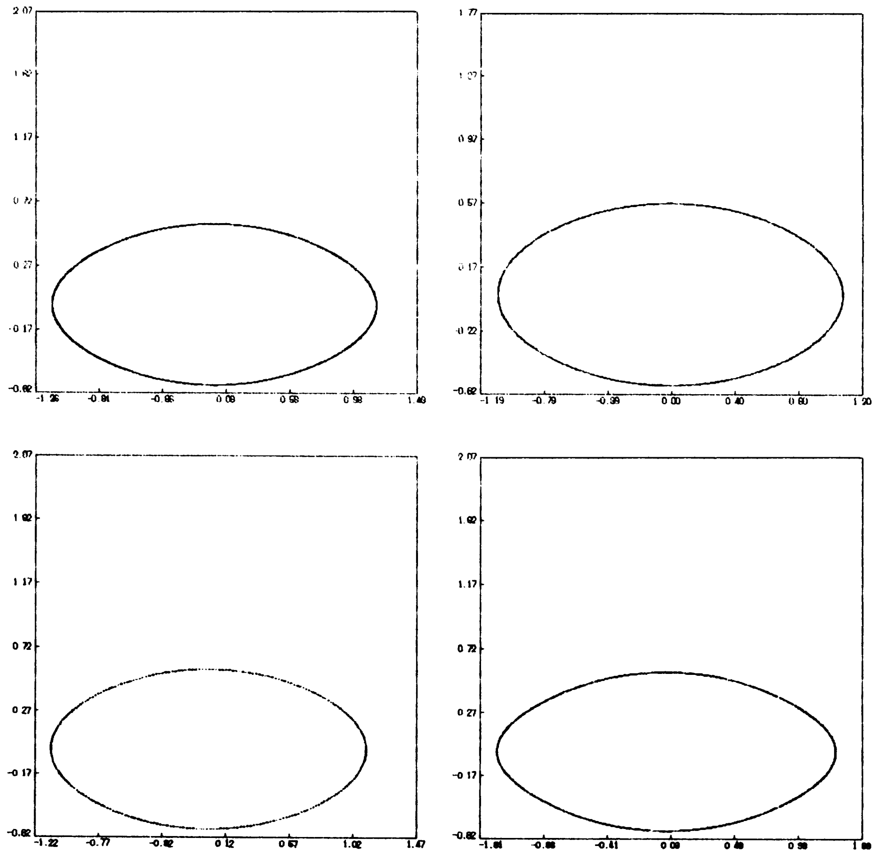


Fig.5. Preservation and breakdown of invariant tori for nonlinear oscillator $H = (p^2 + a^2q^2 + a^4q^4/12)/2, \quad a = 2$.

Explicit symplectic composite scheme, order 2.

stepsize=τ, total number of steps=N, number of steps per plot = M.

Five orbits are computed in all cases with the same set of five initial points.

Upper-left: $\tau = 0.5$, $N = 2000$, $M = 1$. Upper-right: $\tau = 0.1$, $N = 2000$, $M = 1$.

Lower-left: $\tau = 0.3$, $N = 2000$, $M = 1$. Lower-right: $\tau = 0.1$, $N = 1000000$, $M = 500$.

The five initial points are (0.5, 0.25), (0.65, 0.535), (0.375, 0.55), (0.685, 0.65), (0.495, 0.375). For smaller stepsize 0.3671 (upper-left), all the invariant tori are preserved practically, the effect of segmentation is almost imperceptible. However, for larger stepsizes (upper-left, lower-left, lower-right), while some invariant tori are preserved, the breakdown becomes pronounced. Some invariant tori are severely segmented and some are broken down into islands. This phenomenon is typical in the perturbation theory of Hamiltonian dynamics.

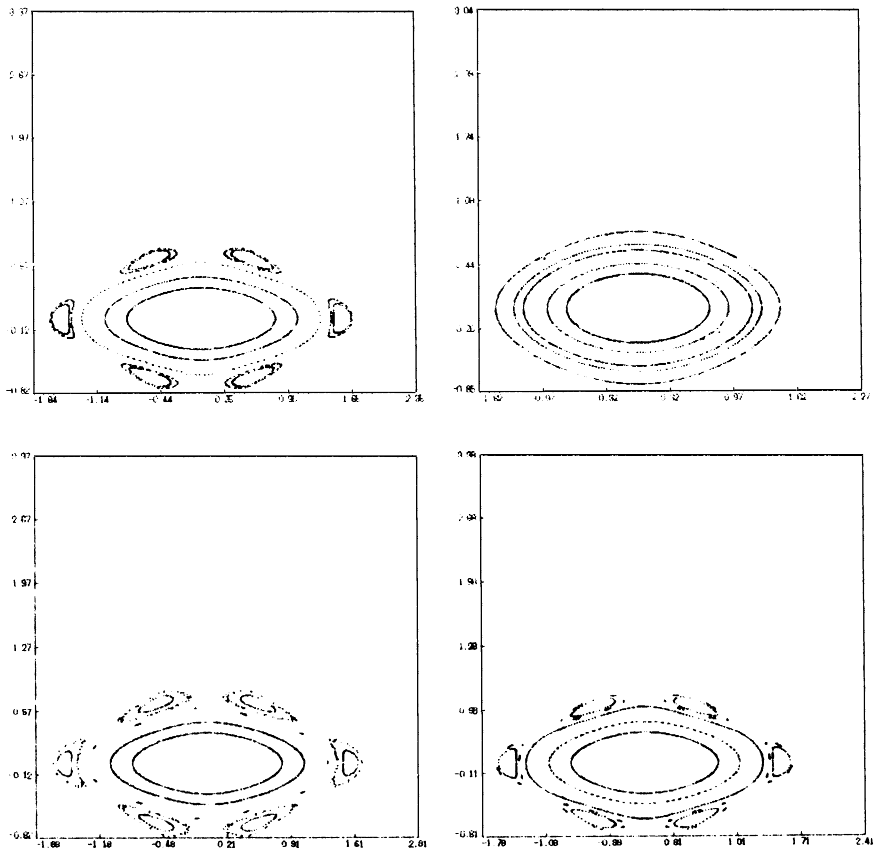


Fig.6. Hamiltonian with 4-fold rotational symmetry, using H_k in (22), $k = 4$.
Explicit symplectic composite scheme, order 2 (21).
stepsize=τ, total number of steps=N, number of steps per plot = M.
Upper-part: $\tau = 1.3$, $N = 10000$, $M = 1$.
Lower-left: $\tau = 0.20000002$, $N = 40000$, $M = 1$. Lower-right: $\tau = 0.2$, $N = 40000$, $M = 1$.

In the symplectic scheme for system with Hamiltonian H_k, the initial point, chosen on or very near to a separatrix, moves within an Arnold web which is a network of canals with the separatrices as its skeleton. The canals become thinner with smaller τ. The separatrix network of H_4 is a square lattice. For larger $\tau = 1.3$ (upper part) the diffusion pattern is more wide-spread and coarse. For small τ the motion is almost rectilinear along the lattice plus random turnings at the crossings, see the cases of $\tau = 0.2$ (lower-right) and $\tau = 0.20000002$ (lower-left), which, in addition, show the extreme sensitivity of the diffusion pattern to the stepsize τ.

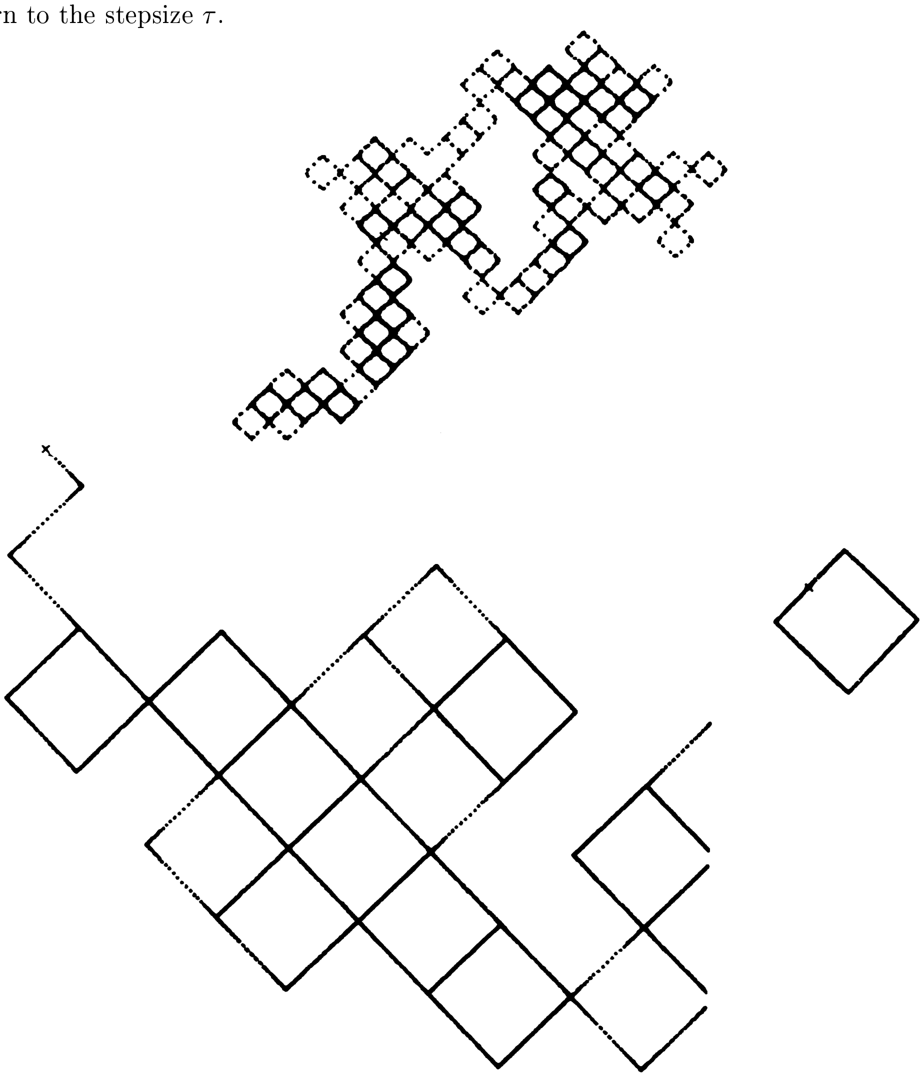


Fig.7. Hamiltonian with 3-fold rotational symmetry, using H_k in (22), $k = 3$.
Explicit symplectic composite scheme, order 2 (21).
stepsize=τ, total number of steps=N, number of steps per plot = M.
Single orbit is computed in all cases.
Upper-left: $\tau = 1.4$, $N = 4000$, $M = 2$. Upper-right: $\tau = 1.04$, $N = 10000$, $M = 1$.
Lower-left: $\tau = 0.7002$, $N = 10000$, $M = 2$. Lower-right: $\tau = 0.7$, $N = 25000$, $M = 5$.

The separatrix network of H_3 (which is proportional to H_6) is a periodic lattice composed of triangles and hexagons. For large $\tau = 1.4$ (upper-left) we get a very coarse web; then at $\tau = 1.04$ (upper-right) the diffusion path is still not fully straightened. For smaller $\tau = 0.7002$ (lower-left) the diffusion is quite uniform and wide-spread. However, with slightly different $\tau = 0.7$ (lower-right), the diffusion behavior becomes grossly different. In an early stage up to 14000 steps the point is confined on an initial triangle, then it moves out to a far away hexagon and stays there again for a long time and then in certain way repeats such oscillating visits between these two entities.

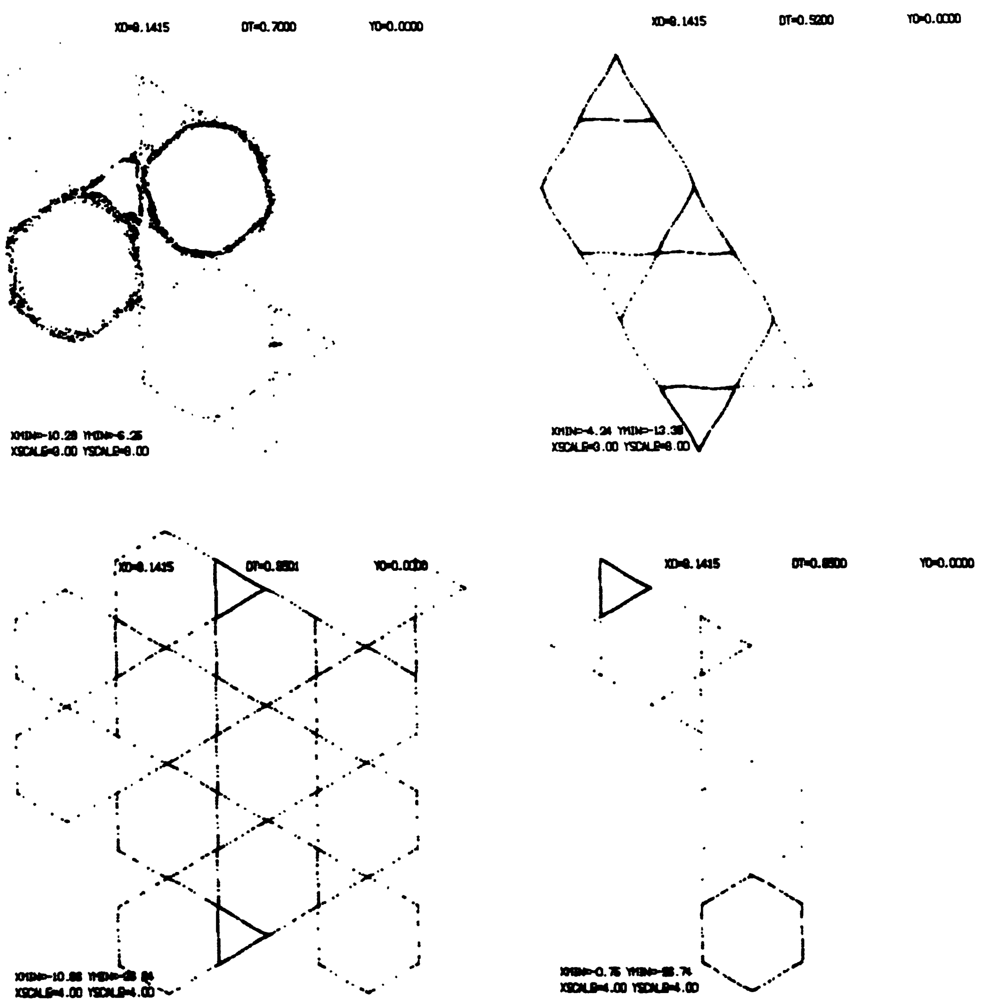
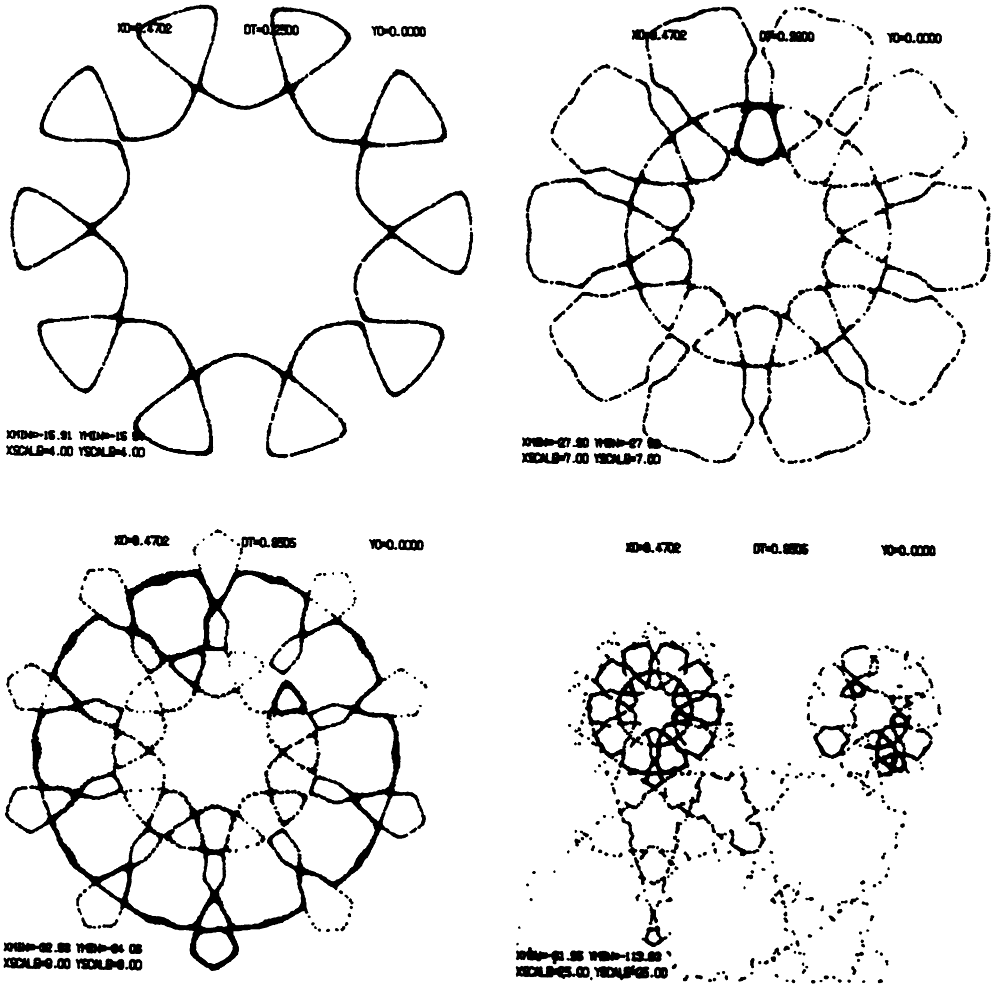


Fig.8. Hamiltonian with 5-fold rotational symmetry, using H_k in (22), $k = 5$.
Explicit symplectic composite scheme, order 2 (21).
stepsize=τ, total number of steps=N, number of steps per plot = M.
Single orbit is computed in all cases.
Upper-left: $\tau = 0.5$, $N = 100000$, $M = 10$. Upper-right: $\tau = 0.56$, $N = 50000$, $M = 5$.
Lower-left: $\tau = 0.701$, $N = 20000$, $M = 1$. Lower-right: $\tau = 0.701$, $N = 100000$, $M = 10$.

The separatrix network of H_5 (proportional to H_{10}) is not periodic but quasiperiodic and not connected, looks like a Penrose tiling with 10-fold symmetry. For small values $\tau = 0.5$ (upper-left) and $\tau = 0.56$ (upper-right) we get trapped diffusion, resulting in rosette patterns with 10-fold symmetry. For larger $\tau = 0.701$ (lower left and right, for evolution) we get the spread-out pattern (see also [21]) which looks like certain Moslem decoration and the electron diffraction pattern of a 2D decagonal quasicrystal, cf. [22].



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