SYMPLECTIC ALGORITHMS FOR HAMILTONIAN SYSTEMS[①]

哈密尔顿系统的辛算法

Abstract

In this paper we give a brief survey on the research, mainly undertaken by the authors and their research group, on various aspects of symplectic algorithms, such as construction of explicit and implicit symplectic algorithms of Hamiltonian systems, conservation laws, linear stability and formal energies.

§1 Introduction

Hamiltonian systems have a fundamental geometry — symplectic geometry. Their phase flow preserves the symplectic geometric structure, which is a one parameter group of symplectic transformations. Different from conventional numerical methods, symplectic algorithms simulate Hamiltonian systems in the same geometric framework, i.e., the step transition operators of symplectic algorithms are symplectic transformations. Hence, they have no artificial excitation and dissipation while most conventional numerical methods inevitably bring in artificial excitation and dissipation. Therefore, symplectic algorithms are pure and clean and suitable to long term tracking and qualitative simulations. The idea has been widely generalized to other systems with geometric structures or Lie algebraic structures, such as contact algorithms for contact systems, volume preserving algorithms for source free systems, which all are named structure preserving algorithms. Readers interested in these aspects can refer to [13, 15, 16, 19, 22, 47].

In this paper we only review symplectic algorithms for Hamiltonian systems, the construction of algorithms, conservation laws, linear stability and formal energies.

In section 2, we give some basic materials of ordinary differential equations and numerical methods. In section 3, we introduce symplectic algorithms for Hamiltonian systems. Section 4 is concerning with symplectically separable Hamiltonian systems and explicit symplectic algorithms. Symplectic algorithms are essentially implicit, but for symplectically separable systems, explicit schemes can be constructed. In section 5 we discuss unconditional symplectic algorithms and the generating function methods. Section 6 is for symplectic algorithms of perturbed Hamiltonian systems. In section 7 symplectic Runge-Kutta methods are given. In section 8, we consider the conservation laws of symplectic algorithms. In

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section 9, we discuss the linear stability of symplectic algorithms — H-stability. Section 10 concerns with formal and non-autonomous perturbed energies of symplectic algorithms.

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§2 Preliminaries

2.1 Phase flow

Consider the autonomous system on $\mathbf{R}^m$

$$\dot{z} = a(z), \quad z = (z_1, \cdots, z_m)^T, \quad a(z) = (a_1(z), \cdots, a_m(z))^T, \tag{2.1}$$

where $a(z)$ is a smooth vector field on $\mathbf{R}^m$. The superscript T denotes transpose of a matrix. The solution of System (2.1) with an initial point $z(0) = z_0$ is denoted by $z(t; z_0) = e_a^t z_0$. Usually, it exists for initial points in a domain $\mathcal{D}$ on $\mathbf{R}^m$ and for time in an interval (a, b) containing 0. For simplicity we assume $\mathcal{D} = \mathbf{R}^m$ and $(a, b) = \mathbf{R}$. The solution $z(t; z_0)$ smoothly depends not only on time t but also on initial points z_0. Hence for any fixed t, e_a^t is a transformation on $\mathbf{R}^m$ and is called the phase flow, or t-flow, of System (2.1).

The phase flow e_a^t of System (2.1) defined by the vector field a satisfies

$$\begin{aligned} &\frac{d}{dt} e_a^t = a \circ e_a^t, \\ &e_a^0 = \text{ identity } := 1_m. \end{aligned}$$

e_a^t is a one parameter group in t

$$\begin{aligned} &e_a^{t+s} = e_a^t \circ e_a^s, \quad \forall t, s \in \mathbf{R}, \\ &e_a^0 = 1_m \end{aligned} \tag{2.2}$$

and expressible as a convergent, at least locally, power series

$$e_a^t = \sum_{k=0}^{\infty} t^k e_k, \tag{2.3}$$

where the coefficients are smooth vector functions from $\mathbf{R}^m$ to $\mathbf{R}^m$ and can be determined recursively

$$e_0 = e^0 = 1_m, \ e_1 = a, \ e_k = \frac{1}{k}(e_{k-1})_* e_1, \quad k = 1, 2, \cdots, \tag{2.4}$$

here Jacobian matrix of $u : \mathbf{R}^m \to \mathbf{R}^m$ is denoted by u_*.

2.2 Numerical methods

We now consider a one-step numerical method to approximate System (2.1). When $z^0 = z_0$ is given, we then can get $z^1, z^2, \cdots$ by the method (explicitly or implicitly). Obviously, z^0 can be taken as any initial point. Therefore, this method really defines a mapping on $\mathbf{R}^m$ with the time step-size, say s, as a parameter, denoted by g_a^s. Thus

$$z^0 \text{ given}, \ z^{k+1} = g_a^s z^k, \qquad k \geq 0.$$

The method is said to be of order $r (\geq 1)$ if

$$g_a^s = e_a^s + O(s^{r+1}). \tag{2.5}$$

Therefore, it is equivalent to consider the approximation of $\{z^k\}$ to $z(ks)$ and of $(g_a^s)^k$ to e_a^{ks}. g_a^s is called the step transition operator (or mapping) of the method (or synonymously, algorithm). We always identify the step transition operator with a numerical method.

For example, the explicit and implicit Euler schemes for System (2.1) are

$$\begin{aligned} z \to \hat{z} = E_a^s z: &\qquad \hat{z} = z + sa(z), \\ z \to \hat{z} = I_a^s z: &\qquad \hat{z} = z + sa(\hat{z}). \end{aligned}$$

Their step transition operators E_a^s and I_a^s are

$$E_a^s = 1_m + sa, \qquad I_a^s = (1_m - sa)^{-1}. \tag{2.6}$$

Two-leg and one-leg weighted Euler schemes are

$$\begin{aligned} z \to \hat{z} = T_{a,c}^s z: &\quad \hat{z} = z + s(ca(\hat{z}) + (1-c)a(z)), \\ z \to \hat{z} = E_{a,c}^s z: &\quad \hat{z} = z + sa(c\hat{z} + (1-c)z), \end{aligned} \tag{2.7}$$

where c is a real number. Their step transition operators $T_{a,c}^s$ and $E_{a,c}^s$ are

$$\begin{aligned} T_{a,c}^s &= (1_m - sca)^{-1} \circ (1_m + s(1-c)a) = I_a^{cs} \circ E_a^{(1-c)s}, \\ E_{a,c}^s &= (1_m + s(1-c)a) \circ (1_m - sca)^{-1} = E_a^{(1-c)s} \circ I_a^{sc}. \end{aligned}$$

These show that $T_{a,c}^s$ and $E_{a,c}^s$ are really the composite schemes of the explicit and implicit schemes, $E_a^{(1-c)s}$ and I_a^{sc}, with different orders. Here the composite method $g^s = g_k^s \circ \cdots \circ g_1^s$ of methods $g_1^s, \cdots, g_k^s$ is implemented by the k-stage

$$z \to \hat{z} = g^s z: \quad z^1 = g_1^s z,\ z^2 = g_2^s z^1,\ \cdots,\ z^{k-1} = g_{k-1}^s z^{k-2},\ \hat{z} = g_k^s z^{k-1}.$$

If $g_1^s, \cdots, g_k^s$ are explicit, then g^s is also explicit.

The transition operator g^s can be expressible as a power series

$$g_a^s = \sum_{k=0}^{\infty} s^k g_k, \quad g_0 = 1_m. \tag{2.8}$$

The order condition (2.5) is equivalent to

$$g_k = e_k, \quad k = 0, 1, \cdots, r; \quad g_{r+1} \neq e_{r+1}. \tag{2.9}$$

2.3 Revertibility

The group property (2.2) of the phase flow is a quite strong property. Usually, a numerical method can not be a group in step size s. Hence we consider a weak property of the phase flow e_a^t.

Let g^t be a one-parameter family of near-1 diffeomorphisms with $g^0 = 1_m$. g^t is called *revertible* if $g^t \circ g^{-t} = 1_m$, $\forall t$. We define the reversion of g^t as

$$\breve{g}^t = \left(g^{-t}\right)^{-1}. \tag{2.10}$$

g^t is revertible if and only if $g^t = \breve{g}^t$. Obviously, phase flow e_a^t is revertible. Moreover, we have

(1) $\breve{g}^t \circ g^t$ and $g^t \circ \breve{g}^t$ are always revertible for all g^t.

(2) $\breve{\breve{g}}^t = g^t$, $(f^t \circ g^t)^\vee = \breve{g}^t \circ \breve{f}^t$.

(3) If f^t and g^t are revertible then $f^{\alpha t} \circ g^{\beta t} \circ f^{\alpha t}$ and $f^{\alpha t} \circ g^{\beta t} \circ g^{\beta t} \circ f^{\alpha t}$ are revertible for all $\alpha, \beta \in \mathbf{R}$.

(4) If f_i^t are revertible, $i = 1, \cdots, k$ then $f_1^{\alpha_1 t} \circ \cdots \circ f_k^{\alpha_k t} \circ f_k^{\alpha_k t} \circ \cdots \circ f_1^{\alpha_1 t}$ are revertible for all $\alpha_i \in \mathbf{R}$, $i = 1, \cdots, k$.

(5) When f^t and g^t are revertible then $f^t \circ g^t$ is revertible if and only if $f^t \circ g^t = g^t \circ f^t$.

It can be seen from (2.6) and (2.7) that $I_a^s = (E_a^{-s})^{-1} = \check{E}_a^s$, i.e., the reversion of the explicit Euler operator is the implicit Euler operator, and $\check{T}_{a,c}^s = T_{a,1-c}^s$, $\check{E}_{a,c}^s = E_{a,1-c}^s$, i.e., the reversion of the two- and one-leg Euler operators with the parameter c are the two- and one-leg Euler operators with the parameter $1 - c$.

Consequently, $T_{a,c}^s$ and $E_{a,c}^s$ are revertible for any vector field a if and only if $c = \frac{1}{2}$, i.e., they are trapezoidal and centered Euler schemes respectively.

2.4 Composition Methods

We write $g^s \approx e_a^s$ if $g^s = e_a^s + O(s^2)$, $g^s \approx e_a^s$, ord r if $g^s = e_a^s + O(s^{r+1})$, $g^s \approx e_a^s$, ord ∞ if $g^s = e_a^s$. A consistent revertible algorithm is always of even order $2l (l \geq 1)$. For $g^s \approx e_a^s$, ord 1,

$$g^{s/2} \circ \check{g}^{s/2} \quad \text{and} \quad \check{g}^{s/2} \circ g^{s/2} \approx e_a^s \tag{2.11}$$

are revertible and of order 2. If $g^s \approx e_a^s$ is revertible and of order 2, then the revertible composite of g^s:

$$g^{\alpha s} \circ g^{\beta s} \circ g^{\alpha s} \approx e_a^s \tag{2.12}$$

is of order 4 when

$$2\alpha + \beta = 1, \quad 2\alpha^3 + \beta^3 = 0, \tag{2.13}$$

i.e.,

$$\alpha = \frac{1}{2 - 2^{1/3}} > 0, \qquad \beta = 1 - 2\alpha < 0.$$

Generally, if $g^s \approx e_a^s$ is revertible and of order $2l$, then the revertible composite (2.12) of g^s is of order $2(l+1)$, when

$$2\alpha + \beta = 1, \quad 2\alpha^{2l+1} + \beta^{2l+1} = 0, \tag{2.14}$$

i.e.,

$$\alpha = \frac{1}{2 - 2^{1/(2l+1)}} > 0, \qquad \beta = 1 - 2\alpha < 0.$$

Since g^s is of order $2l$, there exists a vector function $\bar{e}$ such that

$$g^s = e^s + s^{2l+1}\bar{e} + O(s^{2l+2}).$$

Then

$$\begin{aligned} g^{\beta s} \circ g^{\alpha s} &= (e^{\beta s} + \beta^{2l+1} s^{2l+1} \bar{e}) \circ (e^{\alpha s} + \alpha^{2l+1} s^{2l+1} \bar{e}) + O(s^{2l+2}) \\ &= e^{(\beta+\alpha)s} + (\beta^{2l+1} + \alpha^{2l+1}) s^{2l+1} \bar{e} + O(s^{2l+2}). \end{aligned}$$

Similarly, we have

$$g^{\alpha s} \circ g^{\beta s} \circ g^{\alpha s} = e^{(\beta+2\alpha)s} + (\beta^{2l+1} + 2\alpha^{2l+1}) s^{2l+1} \bar{e} + O(s^{2l+2}).$$

Consequently, Condition (2.14) leads to that

$$g^{\alpha s} \circ g^{\beta s} \circ g^{\alpha s} = e^s + O(s^{2l+2}),$$

i.e., it is of order $2l + 1$. Since it is revertible, it must be of order $2l + 2$.

For more details, refer to [21, 33, 36, 52]

§3 Symplectic Algorithms — A Geometric View-point

We consider now Hamiltonian systems on $\mathbf{R}^{2n}$

$$\begin{aligned} \frac{dp}{dt} &= -H_q, \\ \frac{dq}{dt} &= H_p, \end{aligned} \qquad p = \begin{pmatrix} p_1 \\ \vdots \\ p_n \end{pmatrix}, \quad q = \begin{pmatrix} q_1 \\ \vdots \\ q_n \end{pmatrix},$$

or in compact form,

$$\frac{dz}{dt} = J\nabla H(z), \quad z = \begin{pmatrix} p \\ q \end{pmatrix} \in \mathbf{R}^{2n}, \quad J = J_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix}, \tag{3.1}$$

where $H(z)$ is a Hamiltonian function, $\nabla H(z) = H_z = (H_{z_1}(z), \cdots, H_{z_{2n}}(z))^T$ is the gradient of H with respect to z, 0 and I are the n by n zero and identity matrices. The phase flow of (3.1) is denoted by e_H^t which can be expanded as a power series

$$e_H^t = e_0 + te_1 + t^2 e_2 + \cdots, \tag{3.2}$$

where

$$\begin{aligned} &e_0 = 1_{2n},\ e_1 = J\nabla H,\ e_2 = \frac{1}{2}(J\nabla H)_* J\nabla H, \\ &e_k = \frac{1}{k}(e_{k-1})_* J\nabla H,\ k \geq 3. \end{aligned} \tag{3.3}$$

The symplectic structure on $\mathbf{R}^{2n}$ is defined by the differential 2-form

$$\omega = \sum_{i=1}^{n} dp_i \wedge dq_i$$

which corresponds to the 2-dimensional oriented area on the tangent space of $\mathbf{R}^{2n}$. A *symplectic* transformation is a diffeomorphism $g : z \to \hat{z}$ on $\mathbf{R}^{2n}$ preserving the symplectic structure

$$g^*\omega = \omega \qquad \text{i.e.,} \qquad \sum d\hat{p}_i \wedge d\hat{q}_i = \sum dp_i \wedge dq_i,$$

or in matrix form,

$$g_*^T(z) J_{2n} g_*(z) \equiv J_{2n}.$$

Hence all symplectic transformations automatically preserve phase areas of even dimensions. All symplectic transformations on $\mathbf{R}^{2n}$ form a group under composition of transformations, denoted by SpD_{2n}.

Intrinsic to all Hamiltonian systems is that the phase flow of Hamiltonian systems preserves the symplectic structure, i.e.,

$$(e_H^t)^*\omega = \omega, \qquad \text{or} \qquad (e_H^t)_*^T(z) J (e_H^t)_*(z) = J, \quad \forall z \in \mathbf{R}^{2n}, t \in \mathbf{R}.$$

It follows that the phase areas of even-dimensions and the Hamiltonian (energy) are conserved in time evolution. It is natural and mandatory to require algorithms to be symplectic, such algorithms are called symplectic algorithms. More precisely, symplectic algorithms are numerical methods whose step transition operator g_H^s preserves the symplectic structure of the phase space as applied to Hamiltonian systems, i.e.,

$$(g_H^s)_*^T J (g_H^s)_* = J. \tag{3.4}$$

Hence symplectic algorithms also automatically preserve phase areas of even dimensions.

Conventional numerical methods only consider the accuracy of approximation of numerical solutions to exact solutions. They do not concern with the geometric properties that the systems possess. On the one hand, Hamiltonian systems are conversation systems, while most conventional numerical methods, such as Runge-Kutta methods, have an artificial excitation or dissipation which will completely destroy the behavior of the exact solutions in long term simulation. Symplectic algorithms are clean, they do not have such artificial excitation and dissipation and are able to preserve the behavior of the solution in long term simulation. On the other hand, a system of differential equations is a continuous dynamical system, a numerical method to approximate the system can be regarded as a discrete dynamical system for fixed time step-size. Therefore, when one uses a method to solve a system (problem), one really uses a discrete dynamical system to simulate a continuous dynamical system. In this sense, it is natural to require that the numerical simulation should be done in the same geometric framework, especially in long term tracking and qualitative numerical simulations. This requirement is easy to understand since in long term simulation, any numerical solution is far from the exact solution, only the qualitative properties remain. In this aspect, symplectic algorithms are overwhelmingly superior to conventional numerical methods. This idea has been widely generalized to other systems, such as contact systems, source free systems, Poisson systems, systems with Lie algebraic structures. Readers interested in this field can refer to [13, 15, 16, 19, 22, 47].

§4 Explicit Symplectic Algorithms

There are two kinds of symplectic algorithms. One is called unconditional symplectic algorithms which are symplectic for all Hamiltonian systems, another is symplectic for a kind of Hamiltonians. For example, explicit Euler scheme is generally non-symplectic, but it is symplectic for $H(z) = U(q)$ or $V(p)$. In this section we will construct explicit symplectic algorithms for symplectically separable Hamiltonian systems by composition of explicit Euler schemes.

Definition 1. A Hamiltonian function H is nilpotent of degree 2 if

$$(\nabla H)_* J \nabla H = 0 \quad \text{or} \quad H_{zz} J H_z = 0. \tag{4.1}$$

For Hamiltonians H nilpotent of degree 2, by the expressions (3.2) and (3.3), $e_k = 0$ for $k \geq 2$. Therefore the phase flow is

$$e_H^t(z) = z + te_1(z) = z + tJ\nabla H(z),$$

which is just the explicit Euler scheme at $t = s$: $e_H^s(z) = E_H^s$. So E_H^s must be symplectic. In this case, E_H^s is also revertible since e_H^s is revertible.

Definition 2. $H(z)$ is *symplectically separable* if $H(z)$ can be decomposed as

$$H(z) = \sum_{i=1}^{k} H_i(z) \tag{4.2}$$

and every $H_i(z)$ is nilpotent of degree 2.

For symplectically separable Hamiltonians $H(z)$ with the decomposition (4.2), the following composite

$$z \to \hat{z} = g_1^s z, \quad g_1^s := E_{H_1}^s \circ E_{H_2}^s \circ \cdots \circ E_{H_k}^s \tag{4.3}$$

is explicit, symplectic and of order 1. The symmetric composite

$$\begin{aligned} &z \to \hat{z} = g_2^s z, \\ &g_2^s := g_1^{s/2} \circ \check{g}_1^{s/2} = E_{H_1}^{s/2} \circ \cdots \circ E_{H_{k-1}}^{s/2} \circ E_{H_k}^{s} \circ E_{H_{k-1}}^{s/2} \circ \cdots \circ E_{H_1}^{s/2} \end{aligned} \tag{4.4}$$

is explicit, symplectic and revertible of order 2. Higher order revertible symplectic schemes can be constructed from these schemes by the procedure (2.12), (2.13) and (2.14).

If

$$H(z) = H(p,q) = U(p) \quad \text{or} \quad V(q),$$

where U and V are functions of n variables, then $H(z)$ is nilpotent of degree 2

$$\begin{pmatrix} H_p(p,q) \\ H_q(p,q) \end{pmatrix} = \begin{pmatrix} U_p(p) \\ 0 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 \\ V_q(q) \end{pmatrix}.$$

The corresponding explicit Euler schemes

$$\begin{aligned} &\hat{p} = p \\ &\hat{q} = q + sU_p(p) \end{aligned} \qquad \text{or} \qquad \begin{aligned} &\hat{p} = p - sV_q(q) \\ &\hat{q} = q \end{aligned}$$

are symplectic. If

$$H(p,q) = U(p) + V(q), \tag{4.5}$$

which is symplectically separable, then the composite schemes

$$\begin{aligned} E_V^s \circ E_U^s : &\qquad \hat{p} = p - sV_q(\hat{q}), \qquad \hat{q} = q + sU_p(p), \\ E_U^s \circ E_V^s : &\qquad \hat{p} = p - sV_q(q), \qquad \hat{q} = q + sU_p(\hat{p}) \end{aligned} \tag{4.6}$$

are explicit, symplectic and of order 1. The revertible scheme

$$\begin{aligned} &g_2^s := (E_V^{s/2} \circ E_U^{s/2})^\vee \circ (E_V^{s/2} \circ E_U^{s/2}) = E_U^{s/2} \circ E_V^s \circ E_U^{s/2} : \\ &q^1 = q + \frac{s}{2} U_p(p), \quad \hat{p} = p - sV_q(q_1), \quad \hat{q} = q^1 + \frac{s}{2} U_p(\hat{p}) \end{aligned} \tag{4.7}$$

is symplectic and of order 2. Its revertible composite

$$g_4^s := g_2^{\alpha s} \circ g_2^{\beta s} \circ g_2^{\alpha s}$$

gives an explicit symplectic scheme[24,32,33,36,52] of order 4 with the parameters (2.13), i.e.,

$$\begin{aligned} p^1 &= p - c_1 sV_q(q), & q^1 &= q + d_1 sU_p(p^1), \\ p^2 &= p^1 - c_2 sV_q(q^1), & q^2 &= q^1 + d_2 sU_p(p^2), \\ p^3 &= p^2 - c_3 sV_q(q^2), & q^3 &= q^2 + d_3 sU_p(p^3), \\ \hat{p} &= p^3 - c_4 sV_q(q^3), & \hat{q} &= q^3 + d_4 sU_p(\hat{p}), \end{aligned} \tag{4.8}$$

with the parameters $\alpha = (2 - 2^{1/3})^{-1}$, $\beta = 1 - 2\alpha$ and either

$$c_1 = 0,\ c_2 = c_4 = \alpha,\ c_3 = \beta,\ d_1 = d_4 = \alpha/2,\ d_2 = d_3 = (\alpha + \beta)/2, \tag{4.9}$$

or

$$c_1 = c_4 = \alpha/2, \quad c_2 = c_3 = (\alpha + \beta)/2, \quad d_1 = d_3 = \alpha, \quad d_2 = \beta, \quad d_4 = 0. \tag{4.10}$$

The 3rd order explicit symplectic scheme[37] for the separable Hamiltonian (4.5) is given by

$$\begin{aligned} p^1 &= p - c_1 s V_q(q), & q^1 &= q + d_1 s U_p(p^1), \\ p^2 &= p^1 - c_2 s V_q(q^1), & q^2 &= q^1 + d_2 s U_p(p^2), \\ \hat{p} &= p^2 - c_3 s V_q(q^2), & \hat{q} &= q^2 + d_3 s U_p(\hat{p}) \end{aligned} \tag{4.11}$$

with the parameters

$$c_1 = 7/24,\ c_2 = 3/4,\ c_3 = -1/24,\ d_1 = 2/3,\ d_2 = -2/3,\ d_3 = 1, \tag{4.12}$$

or

$$c_1 = 1,\ c_2 = -2/3,\ c_3 = 2/3,\ d_1 = -1/24,\ d_2 = 3/4,\ d_3 = 7/24. \tag{4.13}$$

Symplectically separable Hamiltonians have wide coverage in applications. It is easy to see that, the Hamiltonian of the form

$$H(p,q) = \phi(Ap + Bq), \quad AB^T = BA^T, \tag{4.14}$$

where $\phi(x)$ is a function of n variables, A and B are $n \times n$ matrices, is also nilpotent of degree 2. The explicit Euler scheme $E_H^s = E^s(\phi) = e_H^s$ is

$$E^s(\phi): \quad \begin{aligned} \hat{p} &= p - sB^T \phi_x(Ap + Bq), \\ \hat{q} &= q + sA^T \phi_x(Ap + Bq). \end{aligned} \tag{4.15}$$

Hence we get a class of symplectically separable Hamiltonians[21]

$$H(p,q) = \sum_{i=1}^{k} H_i(p,q), \quad H_i(p,q) = \phi_i(A_i p + B_i q), \quad A_i B_i^T = B_i A_i^T, \tag{4.16}$$

where $\phi_i(x)$ are functions of n variables, A_i and B_i are $n \times n$ matrices. Moreover, all polynomial Hamiltonians belong to this class; in fact, it has been proved in [21] that every polynomial $H(p,q)$ in $2n$ variables p, q can be decomposed in the form of (4.16) with polynomials $\phi_i(x)$ of n variables x and diagonal matrices $A_i = \mathrm{diag}(a_1^i, \cdots, a_n^i)$ and $B_i = \mathrm{diag}(b_1^i, \cdots, b_n^i)$.

For symplectically separable Hamiltonians of the above class, all explicit revertible symplectic schemes formed by composition contain solely the Euler schemes $E^s(\phi_i)$ in the form (4.15) as basic components.

More generally, if we have a decomposition $H = H_1 + \cdots + H_k$, for which each H_i is integrable and its phase flow $e_{H_i}^s$ is algorithmically implementable, then the symmetrical composites

$$\begin{aligned} g_{2,H}^s &= e_{H_1}^{s/2} \circ \cdots \circ e_{H_{k-1}}^{s/2} \circ e_{H_k}^{s} \circ e_{H_{k-1}}^{s/2} \circ \cdots \circ e_{H_1}^{s/2} \\ g_{4,H}^s &= g_{2,H}^{\alpha s} \circ g_{2,H}^{\beta s} \circ g_{2,H}^{\alpha s} \quad \text{with parameters (2.13)} \end{aligned}$$

give symplectic and revertible algorithms of order 2, 4, etc. This general approach is widely applicable to *many body problems* in different physical contexts for which the *2-body problem* is *solvable*. Since in such problems the Hamiltonian usually admits a natural decomposition $H = \sum_{i<j} H_{ij}$, each H_{ij} accounts for a 2-body problem.

An interesting result from this approach is a construction[55] of explicit symplectic method for computing the Hamiltonian system of N vortices $z_i = (x_i, y_i)$ with intensities k_i

$$k_i \frac{dx_i}{dt} = \frac{\partial H}{\partial y_i}, \qquad k_i \frac{dy_i}{dt} = -\frac{\partial H}{\partial x_i}, \quad i = 1, \cdots, N$$

with symplectic structure $\omega_k = \sum \frac{1}{k_i} dx_i \wedge dy_i$ and

$$H = \sum_{i<j} H_{ij}, \quad H_{ij} = -\frac{1}{2\pi} k_i k_j \ln r_{ij}, \quad r_{ij} = ((x_i - x_j)^2 + (y_i - y_j)^2)^{1/2}.$$

Each H_{ij} accounts for a solvable 2-vortex motion in which both vortices z_i, z_j rotate about their center of vorticity $z = (k_i z_i + k_j z_j)(k_i + k_j)^{-1}$ with the angular velocity $a = (k_i + k_j)/2\pi r_{ij}^2$ if $k_i + k_j \neq 0$ or translate with the linear velocity $(b(y_i - y_j), -b(x_i - x_j))$, $b = k_i/2\pi r_{ij}^2$ if $k_i + k_j = 0$. These simple phase flows $e^{s}_{H_{ij}}$ serve as the basic algorithmic components for successive compositions, resulting in efficient explicit revertible methods, symplectic for this specific system. They are promising in application to incompressible ideal flows for tracking the vortex particles.

§5 Generating Function Methods

Now we consider *unconditional* symplectic algorithms, i.e., they are symplectic for *all* Hamiltonian systems.

We first consider the simplest cases: one-leg weighted Euler scheme

$$\hat{z} = E^{s}_{H,c} z: \quad \hat{z} = z + sJH_z(c\hat{z} + (1-c)z) \tag{5.1}$$

with real number c. It is unconditionally symplectic if and only if $c = \frac{1}{2}$, which corresponds to the *centered Euler scheme*

$$\hat{z} = z + sJH_z(\frac{\hat{z} + z}{2}). \tag{5.2}$$

This illustrates a general situation: apart from some very rare exceptions, the vast majority of conventional schemes are non-symplectic. However, if we allow c in (5.1) to be a real matrix of order $2n$, we get a far-reaching generalization: (5.1) is symplectic if and only if

$$c = \frac{1}{2}(I_{2n} + J_{2n}B), \quad B^T = B, \quad c^T J + Jc = J. \tag{5.3}$$

The simplest and important cases are

$$\begin{aligned}
&C: && c = \tfrac{1}{2} I_{2n}, && \hat{z} = z + sJH_z(\frac{\hat{z} + z}{2}),\\
&P: && c = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, && \begin{aligned} \hat{p} &= p - sH_q(\hat{p}, q),\\ \hat{q} &= q + sH_p(\hat{p}, q), \end{aligned}\\
&Q: && c = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, && \begin{aligned} \hat{p} &= p - sH_q(p, \hat{q}),\\ \hat{q} &= q + sH_p(p, \hat{q}). \end{aligned}
\end{aligned} \tag{5.4}$$

For $H(p,q) = U(p) + V(q)$, the above schemes P and Q reduce to explicit symplectic schemes (4.6).

Scheme (5.1) is revertible of order 2 for $c = \frac{1}{2} I$, this is (5.2). (5.1) is of order 1 for $c \neq \frac{1}{2} I$. Since $\check{E}^{s}_{H,c} = E^{s}_{H,I-c}$, the composites

$$E^{s/2}_{H,c} \circ E^{s/2}_{H,I-c} \quad \text{and} \quad E^{s/2}_{H,I-c} \circ E^{s/2}_{H,c}$$

are symplectic, revertible and of order 2. From these schemes we can get 4th and higher order revertible symplectic schemes by the procedure (2.12), (2.13) and (2.14).

So we get a great variety of simple symplectic schemes of order 1, 2, 4, etc., classified according to type matrices $B \in sm(2n) :=$ space of symmetric matrices of order $2n$, which is a linear space of dimension $2n^2 + n$.

A general methodology to construct unconditional symplectic algorithms is generating function method explained below.

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

$$\alpha^T J_{4n} \alpha = \tilde{J}_{4n}, \quad J_{4n} = \begin{pmatrix} 0 & -I_{2n} \\ I_{2n} & 0 \end{pmatrix}, \qquad \tilde{J}_{4n} = \begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix},$$

$$\alpha = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad \alpha^{-1} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}.$$

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

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

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

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

where $Sp(2n) = \left\{ S \in GL(2n, \mathbf{R}) |\ S^T J_{2n} S = J_{2n} \right\}$ is the group of symplectic matrices.

The above machinery can be extended to generally non-linear operators on $\mathbf{R}^{2n}$. Denote $symm(2n)$ the space of symmetric operators on $\mathbf{R}^{2n}$ (not necessary one-one). Every $f \in symm(2n)$ corresponds, at least locally, to a real function ϕ (unique up to a constant) such that f is the gradient of ϕ: $f(w) = \nabla\phi(w)$, where $\nabla\phi(w) = (\phi_{w_1}(w), \cdots, \phi_{w_{2n}}(w))^T = \phi_w(w)$. Then we have

$$\begin{aligned} \sigma_\alpha : \quad & SpD_{2n} \to symm(2n), \\ & \sigma_\alpha(g) = (a \circ g + b) \circ (c \circ g + d)^{-1} = \nabla\phi, \quad \text{for} \quad |cg_z + d| \neq 0, \end{aligned}$$

or alternatively

$$ag(z) + bz = (\nabla\phi)(cg(z) + dz),$$

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

$$\begin{aligned} & \sigma_\alpha^{-1} : \quad symm(2n) \to SpD_{2n}, \\ & \sigma_\alpha^{-1}(\nabla\phi) = (a_1 \circ \nabla\phi + b_1) \circ (c_1 \circ \nabla\phi + d_1)^{-1} = g, \text{ for } |c_1 \phi_{ww} + d_1| \neq 0 \end{aligned} \tag{5.5}$$

or alternatively

$$a_1 \nabla\phi(w) + b_1(w) = g(c_1 \nabla\phi(w) + d_1 w), \tag{5.6}$$

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

For the study of symplectic difference scheme 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

$$\alpha = \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} J & -J \\ c & I-c \end{pmatrix}, \quad c = \frac{1}{2}(I+JB), \quad B^T = B, \tag{5.7}$$

$$\alpha^{-1} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = \begin{pmatrix} (c-I)J & I \\ cJ & I \end{pmatrix}. \tag{5.8}$$

The fractional transform induced by a normal Darboux matrix establishes a 1-1 correspondence between *symplectic operators near identity* and *symmetric operators near nullity*.

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

$$\nabla\phi_{H,\alpha}^t = (Je_H^t - J)\circ(ce_H^t + I - c)^{-1}, \quad \text{for small} \quad |t|. \tag{5.9}$$

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

$$\frac{\partial}{\partial t}\phi(w,t) = -H(w + a_1\nabla\phi(w,t)) = -H(w + c_1\nabla\phi(w,t)) \tag{5.10}$$

and can be expressed by Taylor series in t

$$\phi(w,t) = \sum_{k=1}^{\infty}\phi^{(k)}(w)t^k, \quad |t| \quad \text{small}. \tag{5.11}$$

The coefficients can be determined recursively

$$\begin{aligned} \phi^{(1)}(w) &= -H(w), \quad \text{and for} \quad k \geq 0, \quad a_1 = (c-I)J: \\ \phi^{(k+1)}(w) &= \frac{-1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{j_1+\cdots+j_m=k \\ j_i\geq 1}} D^m H(a_1\nabla\phi^{(j_1)}, \cdots, a_1\nabla\phi^{(j_m)}), \end{aligned} \tag{5.12}$$

where we use the notation of the m-linear form

$$\begin{aligned} &D^m H(w)(a_1\nabla\phi^{(j_1)}(w), \cdots, a_1\nabla\phi^{(j_m)}(w)) \\ &:= \sum_{i_1,\cdots,i_m=1}^{2n} H_{z_{i_1}\cdots z_{i_m}}(w)(a_1\nabla\phi^{(j_1)}(w))_{i_1}\cdots(a_1\nabla\phi^{(j_m)}(w))_{i_m}. \end{aligned}$$

By (5.9), the phase flow $\hat{z} := e_H^t z$ satisfies

$$\begin{aligned} \hat{z} - z &= -J\nabla\phi_{H,\alpha}^t(c\hat{z} + (I-c)z) \\ &= -\sum_{j=1}^{\infty} t^j J\nabla\phi^{(j)}(c\hat{z} + (I-c)z). \end{aligned} \tag{5.13}$$

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

$$g^s = \sigma_\alpha^{-1}(\nabla\psi^s), \quad |s| \quad \text{small}, \tag{5.14}$$

which depends on s, H, α (or equivalently B) and the mode of truncation. It is a symplectic approximation to the phase flow e_H^s and can serve as the transition operator of a symplectic difference scheme (for the Hamiltonian system (3.1))

$$z \to \hat{z} = g^s z: \quad \hat{z} = z - J\nabla\psi^s(c\hat{z} + (I-c)z), \quad c = \frac{1}{2}(I+JB). \tag{5.15}$$

Thus, using the machinery of phase flow generating functions we have constructed, for every H and every normal Darboux matrix α, a hierarchy of symplectic schemes by truncation. The simple symplectic schemes (5.4) correspond to the lowest truncation.

§6 Hamiltonian Algorithms for Hamiltonian Systems with a Perturbation Parameter

The machinery above can also be applied to construct symplectic algorithms for perturbed Hamiltonian systems defined by the perturbed Hamiltonian

$$H(z;\epsilon) = \sum_{k=0}^{\infty} \epsilon^k H_k(z) = H_0(z) + \sum_{k=1}^{\infty} \epsilon^k H_k(z), \tag{6.1}$$

where ϵ is the small perturbation parameter. $H_0(z)$ is usually an integrable Hamiltonian. The corresponding perturbed Hamiltonian system is

$$\frac{dz}{dt} = JH_z(z,\epsilon), \qquad z \in \mathbf{R}^{2n}. \tag{6.2}$$

Its phase flow, denoted by $e_\epsilon^t = e_{H,\epsilon}^t$, depends on the parameter ϵ. The Hamilton-Jacobi equation and generating function are also parameterized by ϵ. That means, the parameterized generating function $\phi_\epsilon^t(w) = \phi^t(w,\epsilon) = \phi(w,t,\epsilon)$ satisfies the parameterized Hamilton-Jacobi equation

$$\frac{\partial}{\partial t}\phi(w,t,\epsilon) = -H(w + a_1\nabla\phi(w,t,\epsilon),\epsilon). \tag{6.3}$$

$\phi(w,t,\epsilon)$ can be expanded as a power series in ϵ in stead of t

$$\phi(w,t;\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \phi^{(k)}(w,t). \tag{6.4}$$

The coefficients $\phi^{(k)}(w,t)$ satisfy the following equations:

$$\phi_t^{(0)}(w,t) = -H_0(w + a_1\nabla\phi^{(0)}(w,t)), \tag{6.5}$$

$$k \geq 1: \ \phi_t^{(k)}(w,t) = -H_k(w^*) - \sum_{i=1}^{k}\sum_{m=1}^{i} \frac{1}{m!} \sum_{\substack{i_1+\cdots+i_m=i \\ i_j \geq 1}} D^m H_{k-i}(w^*) \times (a_1\nabla\phi^{(i_1)}(w,t), \cdots, a_1\nabla\phi^{(i_m)}(w,t)) \tag{6.6}$$

with the initial points $\phi^{(i)}(w,0) = 0$, where $w^* = w + a_1\nabla\phi^{(0)}(w,t)$.

(6.5) is just the Hamilton-Jacobi equation for the unperturbed Hamiltonian system with Hamiltonian $H_0(z)$. The right hand side of (6.6) can be written as

$$-DH_0(w^*) \cdot a_1\nabla\phi^{(k)}(w,t) + R^{(k)}(w,t),$$

where the remainder $R^{(k)}(w,t)$ depends only on $H_i(w^*)$, $i = 0,1,\cdots,k$ and $\phi^{(i)}(w,t)$, $i = 0,1,\cdots,k-1$. Once $\phi^{(0)}(w,t),\cdots,\phi^{(k-1)}(w,t)$ are known, $R^{(k)}(w,t)$ is also known. Therefore, if $\phi^{(0)}(w,t)$ can be solved from (6.5), then for $k \geq 1$,

$$\phi_t^{(k)}(w,t) = -DH_0(w^*) \cdot a_1\nabla\phi^{(k)}(w,t) + R^{(k)}(w,t)$$

are the linear partial differential equations for $\phi^{(k)}(w,t)$. They have the same coefficients, only those for $R^{(k)}(w,t)$ are different.

In some cases, we can solve (6.5) easily, refer to [45]. In general, it is difficult to solve (6.5) by analytical method. Nevertheless we can always give an approximative solution, for example, using the methods discussed above.

Let now $\psi_\epsilon^s(w) = \psi(w, s, \epsilon)$ be a truncation of $\phi(w, s, \epsilon)$ up to a certain power ϵ^m. Using the inverse transform σ_α^{-1} we get the symplectic operator

$$g_\epsilon^s = \sigma_\alpha^{-1}(\nabla\psi_\epsilon^s), \quad |s| \quad \text{small}. \tag{6.7}$$

It is a symplectic approximation to the phase flow e_ϵ^s of order m in ϵ and can serve as the transition operator of a symplectic difference scheme for the perturbed Hamiltonian system (6.2)

$$z \to \hat{z} = g_\epsilon^s z: \quad \hat{z} = z - J\nabla\psi(c\hat{z} + (I-c)z, s, \epsilon), \quad c = \frac{1}{2}(I + JB). \tag{6.8}$$

For general perturbed Hamiltonians $H(z, \epsilon)$, these schemes are only consistent in the time stepsize s. But for the perturbed Hamiltonians with the form

$$H(z, \epsilon) = H_0(z) + \epsilon H_1(z), \tag{6.9}$$

the order of Scheme (6.8) in the time stepsize s is the same as in ϵ. More precisely, for the m-th order scheme g_ϵ^s for the perturbed Hamiltonian (6.9),

$$g_\epsilon^s = e_\epsilon^s + O\big((s\epsilon)^{m+1}\big). \tag{6.10}$$

Therefore, for small ϵ the time stepsize s can be taken quite large. For more details, refer to [45].

§7 Symplectic Runge-Kutta Methods

For System (2.1) of differential equations, a r-stage Runge-Kutta method is defined by the following procedure

$$\begin{aligned} k_i &= z + s\sum_{j=1}^{r} d_{ij}a(k_j), \quad 1 \le i \le r \\ \hat{z} &= z + s\sum_{j=1}^{r} b_j a(k_j), \end{aligned} \tag{7.1}$$

where d_{ij} and b_j are constants. The parameters d_{ij} and b_j characterize Runge-Kutta methods, which are chosen by order condition.

For Hamiltonian systems, Runge-Kutta methods are usually not symplectic. But if d_{ij} and b_j satisfy the condition

$$M_{ij} = b_i d_{ij} + b_j d_{ji} - b_i b_j \equiv 0 \quad (1 \le i, j \le r) \tag{7.2}$$

then they are symplectic[30,38]. In this case, the methods are implicit. The r-stage Gauss-Legendre methods satisfy Condition (7.2). They have the $2r$-th order of accuracy. The simplest one is

$$d_{11} = \frac{1}{2}, \quad b_1 = 1,$$

which gives

$$k_1 = J\nabla H(z + \frac{s}{2}k_1), \quad \hat{z} = z + sk_1.$$

This is just the centered Euler scheme (or midpoint rule)

$$\hat{z} = z + \frac{s}{2} J\nabla H(\frac{\hat{z}+z}{2}).$$

§8 Conservation Laws

Conservation laws we refer to here have two meanings. As is well known, the Hamiltonian system (3.1) itself has first integrals which are conserved in time evolution, e.g., the Hamiltonian is always a first integral. Hence, the first question is how many first integrals of Hamiltonian system (3.1) can be preserved by symplectic algorithms. The second question is whether or not there exist their own first integrals in case the original first integrals can not be preserved by symplectic algorithms.

8.1 Conservation laws

We first consider preservation of the first integrals of Hamiltonian systems by symplectic algorithms. For detailed discussion, refer to [28, 20, 4].

Consider the Hamiltonian system

$$\frac{dz}{dt} = J\nabla H(z). \tag{8.1}$$

Suppose

$$\hat{z} = g_H^s(z) \tag{8.2}$$

is a symplectic algorithm. Under a symplectic transformation $z = S(y)$, System (8.1) can be transformed into

$$\frac{dy}{dt} = J\nabla \tilde{H}(y), \tag{8.3}$$

where $\tilde{H}(y) = H(S(y))$ and Scheme (8.2) can be transformed into

$$\hat{y} = S^{-1} \circ g_H^s \circ S(y). \tag{8.4}$$

On the other hand, the algorithm g^s can apply to System (8.3) directly and the corresponding scheme is

$$\hat{y} = g_{\tilde{H}}^s(y). \tag{8.5}$$

Naturally, one can ask if (8.4) and (8.5) are the same. This introduces the following concept.

Definition 3. A symplectic algorithm g^s is invariant under the group $\mathcal{G}$ of symplectic transformations, or $\mathcal{G}$-invariant, for Hamiltonian H if

$$S^{-1} \circ g_H^s \circ S = g_{H\circ S}^s, \qquad \forall S \in \mathcal{G};$$

g^s is symplectic invariant for Hamiltonian H if

$$S^{-1} g_H^s \circ S = g_{H\circ S}^s, \qquad \forall S \in Sp(2n).$$

In practice, the second case is more common. Generally speaking, numerical algorithms depend on coordinates, i.e., they are locally represented. But many numerical algorithms may be independent of linear coordinate transformations.

Theorem 4. *Suppose F is a first integral of the Hamiltonian system* (8.1) *and e_F^t is the corresponding phase flow. Then F is conserved up to a constant by the symplectic algorithm g_H^s*

$$F \circ g_H^s = F + c \quad c \text{ is a constant} \tag{8.6}$$

if and only if g_H^s is e_F^t-invariant.

Proof. We first assume that the symplectic algorithm g_H^s is e_F^t-invariant, i.e.,

$$e_F^{-t} \circ g_H^s \circ e_F^t = g_{H \circ e_F^t}^s, \quad \forall t \in \mathbf{R}. \tag{8.7}$$

Since F is a first integral of the Hamiltonian system (8.1) with the Hamiltonian H, H is also the first integral of the Hamiltonian system with the Hamiltonian F, i.e.,

$$H \circ e_F^t = H. \tag{8.8}$$

It follows from (8.7) and (8.8) that

$$e_F^{-t} \circ g_H^s \circ e_F^t = g_H^s,$$

i.e.,

$$e_F^t = (g_H^s)^{-1} \circ e_F^t \circ g_H^s. \tag{8.9}$$

Differentiating (8.9) with respect to t at point 0 and noticing that

$$\left.\frac{de_F^t}{dt}\right|_{t=0} = J\nabla F,$$

we get

$$J\nabla F = (g_H^s)_*^{-1} J\nabla F \circ g_H^s. \tag{8.10}$$

Since g_H^s is symplectic, i.e.,

$$(g_H^s)_*^{-1} J = J(g_H^s)_*^T,$$

we have

$$J\nabla F = J(g_H^s)_*^T \nabla F \circ g_H^s = J\nabla(F \circ g_H^s).$$

Then

$$\nabla F = (g_H^s)_*^T \nabla F \circ g_H^s = \nabla(F \circ g_H^s).$$

It follows that

$$F \circ g_H^s = F + c. \tag{8.11}$$

We now assume that F is conserved by g_H^s, i.e., (8.6) is valid. Then noticing that the phase flows of the vector fields $J\nabla F$ and $(g_H^s)_*^{-1} J\nabla F \circ g_H^s$ are e_F^t and $(g_H^s)^{-1} \circ e_F^t \circ g_H^s$ respectively, we can get (8.7) similarly, i.e., g_H^s is e_F^t-invariant.

Symplectic invariant algorithms are invariant under the symplectic group $Sp(2n)$ and therefore invariant under the phase flow of any quadratic Hamiltonians.

Corolary 5. *Symplectic invariant algorithms for Hamiltonian systems preserve all quadratic first integrals of the original Hamiltonian systems up to a constant.*

If a symplectic scheme has a fixed point, i.e., there is a point z such that $g_H^s(z) = z$, then the constant $c = 0$ and the first integral is conserved exactly. Since linear schemes always have the fix point 0, we then have the following result.

Corolary 6. *Linear symplectic invariant algorithms for linear Hamiltonian systems preserve all quadratic first integrals of the original Hamiltonian systems.*

Example 1. Centered Euler scheme and symplectic Runge-Kutta methods are symplectic invariant. Hence they preserve all quadratic first integrals of System (8.1) up to a constant.

Example 2. Explicit symplectic schemes (4.6), (4.7), (4.11) and (4.8) are invariant under the linear symplectic transformations of the form $\mathrm{diag}\,(A^{-T}, A)$, $A \in GL(n)$. Thus they preserve angular momentum $p^T Bq$ of the original Hamiltonian systems since their infinitesimal symplectic matrices are $\mathrm{diag}\,(-B^T, B)$, $B \in gl(n)$.

In fact, these results can be improved. Symplectic Runge-Kutta methods preserve all quadratic first integrals of System (8.1) exactly[4]. For generating function methods, we have the following result[20].

Theorem 7. *Let $g^s_{H,\alpha}$ be a symplectic method constructed by the generating function method* (5.15) *with the Darboux type α. If $F(z) = \frac{1}{2} z^T Az$, $A \in sm(2n)$, is a quadratic first integral of the Hamiltonian system* (8.1) *and*

$$AJB - BJA = 0, \tag{8.12}$$

then $F(z)$ is conserved by $g^s_{H,\alpha}$, i.e.,

$$F(\hat{z}) = F(z), \quad \textit{or} \quad F \circ g^s_{H,\alpha} = F. \tag{8.13}$$

For $B = 0$, i.e., the case of centered symplectic difference schemes, (8.12) is always valid. So all centered symplectic difference schemes preserve all quadratic first integrals of the Hamiltonian system (8.1) exactly.

Proof. Since $F(z)$ is the first integral of System (8.1),

$$\frac{1}{2}\hat{z}^T A\hat{z} = \frac{1}{2} z^T Az, \quad \hat{z} = e^t_H.$$

It can be rewritten as

$$\frac{1}{2}(\hat{z} + z)^T A(\hat{z} - z) = 0, \quad \hat{z} = e^t_H. \tag{8.14}$$

From (8.12) it follows that

$$\frac{1}{2}\big(JB(\hat{z} - z)\big)^T A\big(\hat{z} - z\big) = \frac{1}{4}\big(\hat{z} - z\big)^T (AJB - BJA)\big(\hat{z} - z\big) = 0, \quad \forall \hat{z}, z \in \mathbf{R}^{2n}.$$

Combining it with (8.14), we have

$$(c\hat{z} + (I - c)z)^T A(\hat{z} - z) = 0.$$

Using (5.13), it becomes

$$(c\hat{z} + (I - c)z)^T AJ \sum_{j=1}^{\infty} t^j \nabla \phi^{(j)}(c\hat{z} + (I - c)z) = 0.$$

From this we get

$$w^T AJ \nabla \phi^{(j)}(w) = 0, \qquad \forall j \geq 1,\ \forall w \in \mathbf{R}^{2n}.$$

Taking $w = c\hat{z} + (I - c)z$, where

$$\hat{z} = g^s_{H,\alpha} z = z - J\nabla \psi^{(m)}(c\hat{z} + (I - c)z) = z - \sum_{j=1}^{m} s^j J \nabla \phi^{(j)}(c\hat{z} + (I - c)z),$$

we have

$$w^T A(\hat{z}-z) = -\sum_{j=1}^{m} s^j\, w^T AJ\nabla\phi^{(j)}(w) = -AJ\nabla\psi(w) = 0.$$

Since

$$\begin{aligned} w^T A(\hat{z}-z) &= \frac{1}{2}\hat{z}^T A\hat{z} - \frac{1}{2}z^T Az + \frac{1}{2}(\hat{z}-z)^T(AJB - BJA)(\hat{z}-z) \\ &= \frac{1}{2}\hat{z}^T A\hat{z} - \frac{1}{2}z^T Az, \end{aligned}$$

it leads to that $F(z)$ is the quadratic invariant of $g^s_{H,\alpha}$.

We list some of the most important normal Darboux's matrices c, the type matrices B, together with the corresponding form of symmetric matrices A of the conserved quadratic invariants $F(z) = \frac{1}{2}z^T Az$:

$$c = I - c = \frac{1}{2}I, \quad B = 0, \quad A \text{ arbitrary.}$$

$$c = \begin{pmatrix} I_n & 0 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & -I_n \\ -I_n & 0 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & b \\ b^T & 0 \end{pmatrix}, \quad b \text{ arbitrary;}$$

$$c = \begin{pmatrix} 0 & 0 \\ 0 & I_n \end{pmatrix}, \quad B = \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix}, \quad \text{angular momentum type.}$$

$$c = \frac{1}{2}\begin{pmatrix} I_n & \pm I_n \\ \mp I_n & I_n \end{pmatrix}, \quad B = \mp I_{2n}, \quad A = \begin{pmatrix} a & b \\ -b & a \end{pmatrix}, \quad a^T = a,\ b^T = -b; \quad \text{Hermitian type.}$$

$$c = \frac{1}{2}\begin{pmatrix} I & \pm I \\ \pm I & I \end{pmatrix}, \quad B = \pm\begin{pmatrix} I_n & 0 \\ 0 & -I_n \end{pmatrix}, \quad A = \begin{pmatrix} a & b \\ -b & -a \end{pmatrix}, \quad \begin{matrix} a^T = a, \\ b^T = -b. \end{matrix}$$

8.2 Conservation laws of linear symplectic algorithms

Apart from the first integrals of the original Hamiltonian systems, a linear symplectic algorithm has its own quadratic first integrals[44]. For the linear Hamiltonian system

$$\frac{dz}{dt} = Lz, \qquad L = JA \in sp(2n) \tag{8.15}$$

with a quadratic Hamiltonian $H(z) = \frac{1}{2}z^T Az$, $A^T = A$, denote its linear symplectic algorithm by

$$\hat{z} = g^s_H(z) = G(s,A)z, \quad G \in Sp(2n). \tag{8.16}$$

Assume that Scheme (8.16) is of order r. Then $G(s)$ has the form

$$\begin{aligned} G(s) &= I + sL(s), \\ L(s) &= L + \frac{s}{2!}L^2 + \frac{s^2}{3!}L^3 + \cdots + \frac{s^{r-1}}{r!}L^r + O(s^r). \end{aligned}$$

For sufficiently small time step size s, $G(s)$ can be represented as

$$G(s) = e^{s\widetilde{L}(s)}, \qquad \widetilde{L}(s) = L + O(s^r), \quad \widetilde{L}(s) \in sp(2n).$$

So (8.16) becomes

$$\hat{z} = e^{s\widetilde{L}(s)}z.$$

This is the solution $z(t)$ of the linear Hamiltonian system

$$\frac{dz}{dt} = \widetilde{L}(s)z, \qquad \widetilde{L}(s) \in sp(2n) \tag{8.17}$$

with the initial value $z(0) = z^0$ evaluated at time s. The symplectic numerical solution

$$z^k = G^k(s)z^0 = e^{ks\widetilde{L}(s)}z^0$$

is just the solution of System (8.17) at discrete points ks, $k = 0, \pm 1, \pm 2, \cdots$. Hence, for sufficiently small s, Scheme (8.16) corresponds to a perturbed linear Hamiltonian system (8.17) with the Hamiltonian

$$\widetilde{H}(z,s) = \frac{1}{2}(z, J^{-1}\widetilde{L}(s)z) = \frac{1}{2}z^T J^{-1}Lz + O(s^r) = H(z) + O(s^r). \tag{8.18}$$

It is well-known that the linear Hamiltonian system (8.17) has n functionally independent quadratic first integrals. So does Scheme (8.16). The following

$$\widetilde{H}_i(z,s) = \frac{1}{2}z^T J^{-1}\widetilde{L}^{2i-1}(s)z, \qquad i = 1, 2, \cdots, n \tag{8.19}$$

are the first integrals of the perturbed system (8.17), therefore, of Scheme (8.16), which approximate the first integrals of System (8.15)

$$H_i(z) = \frac{1}{2}z^T J^{-1}L^{2i-1}z, \qquad i = 1, 2, \cdots, n$$

up to $O(s^r)$. Another group of first integrals of (8.16) is

$$\widehat{H}_i(z,s) = z^T J^{-1}G^i(s)z, \qquad i = 1, 2, \cdots, n.$$

They can be checked easily. The first one is

$$\begin{aligned} \widehat{H}_1(z,s) &= z^T J^{-1}G(s)z = z^T J^{-1}(I + sL(s))z \\ &= sz^T J^{-1}L(s)z = 2sH(z) + O(s^3). \end{aligned}$$

§9 H-stability of Symplectic Algorithms

We know that Hamiltonian systems always appear in spaces of even dimensions. A more important fact is that there is no asymptotically stable linear Hamiltonian system. They are either Liapunov stable or unstable. So are linear symplectic algorithms. Therefore, usual stability concepts in numerical methods for ODE's are not suitable to symplectic algorithms for Hamiltonian systems, for example, A-stability and A(α)-stability, $\alpha < \pi/2$. Hence, usual A(α)-stability is useless for $\alpha < \pi/2$ and A-stability needs to be modified. In this section we discuss the linear stability of symplectic algorithms. Here we introduce a new test system and a new concept — H-stability (Hamiltonian stability) for symplectic algorithms and discuss the H-stability of symplectic invariant algorithms and the H-stability intervals of some explicit symplectic algorithms.

9.1 H-stability of symplectic algorithms

For the linear Hamiltonian system (8.15), a linear symplectic algorithm

$$z^{k+1} = g_H^s(z^k) = G(s, A)z^k, \quad k \geq 0 \tag{9.1}$$

is stable if $\exists C > 0$, such that

$$\|z^k\| = \|G^k(s, A)z^0\| \leq C\|z^0\|, \quad \forall k > 0,$$

where $\|\cdot\|$ is a well defined norm, such as Euclidean norm. Evidently, it is equivalent to $\|G^k(s)\|$ bounded, or, the eigenvalues of $G(s)$ are in the unit disk and its elementary divisors corresponding to the eigenvalues on the unit circle are linear. Since $G(s)$ is symplectic, then

$$G^{-1}(s) = J^{-1}G(s)^T J.$$

Hence if λ is an eigenvalue of $G(s)$, so is λ^{-1}, and they have the same elementary divisors. Therefore, the eigenvalue with the module less than 1 is always accompanied with the eigenvalue with the module great than 1. This implies that the linear symplectic method (9.1) can not be asymptotically stable. It also follows that the linear symplectic method (9.1) is stable if and only if the eigenvalues of $G(s)$ are unimodular and their elementary divisors are linear.

Herein we introduce the test Hamiltonian system

$$\frac{dz}{dt} = \alpha J z, \quad z \in R^2, \quad \alpha \in R \tag{9.2}$$

with the test Hamiltonian

$$H(z) = H(p, q) = \frac{\alpha}{2} z^T z = \frac{\alpha}{2}(p^2 + q^2), \quad A = \alpha I. \tag{9.3}$$

Definition 8. A symplectic difference method is H-stable at $\mu = \alpha s$ if it is stable for the test Hamiltonian system (9.2) with the given μ. Such μ is called a stable point. The maximum interval in which every point is stable and which contains the original point is called the H-stability interval of the method. A symplectic difference method is H-stable if its H-stability interval is the whole real axis, $(-\infty, \infty)$. In this case, its numerical solutions are bounded for (9.2) with $\alpha \in \mathbf{R}$.

On the one hand, the test Hamiltonian (9.3) is the simplest in linear Hamiltonian systems; on the other hand, any stable linear Hamiltonian system has a normal form $H(p, q) = \frac{1}{2}\sum_{i=1}^{n} \alpha_i(p_i^2 + q_i^2)$ under symplectic transformations (see [2, 31, 48]). So the Hamiltonian (9.3) is also general enough. This shows that it is reasonable to take the Hamiltonian system (9.3) as a test system.

For the test system (9.2), (9.1) becomes

$$z^{k+1} = G(\mu)z^k, \tag{9.4}$$

where $G(\mu)$ is a 2×2 symplectic matrix. Denote

$$G(\mu) = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix}.$$

Then $\det G(\mu) = a_1 a_4 - a_2 a_3 = 1$. Its characteristic polynomial is

$$|G(\mu) - \lambda I| = \begin{vmatrix} a_1 - \lambda & a_2 \\ a_3 & a_4 - \lambda \end{vmatrix} = \lambda^2 - (a_1 + a_4)\lambda + 1.$$

So its eigenvalues are

$$\lambda_{\pm} = \frac{a_1 + a_4}{2} \pm \sqrt{(\frac{a_1 + a_4}{2})^2 - 1}.$$

Lemma 9. (9.4) *is stable at* $\mu \neq 0$ *if and only if*

$$(\frac{a_1 + a_4}{2})^2 < 1 \quad or \quad -1 < \frac{a_1 + a_4}{2} < 1. \tag{9.5}$$

Applying the centered Euler scheme to the test system (9.3), it becomes

$$\hat{z} = z + \frac{1}{2}\mu J(\hat{z} + z), \qquad \mu = \alpha s,$$

i.e.,

$$\hat{z} = (I + \frac{1}{2}\mu J)^{-1}(I - \frac{1}{2}\mu J)z,$$

where

$$G(\mu) = (I + \frac{1}{2}\mu J)^{-1}(I - \frac{1}{2}\mu J) = \frac{1}{1 + \frac{1}{4}\mu^2}\begin{pmatrix} 1 - \frac{1}{4}\mu^2 & -\mu \\ \mu & 1 - \frac{1}{4}\mu^2 \end{pmatrix}.$$

So

$$\left(\frac{a_1 + a_4}{2}\right)^2 = \left(\frac{1 - \frac{1}{4}\mu^2}{1 + \frac{1}{4}\mu^2}\right)^2 < 1, \quad \text{for} \quad \mu \neq 0.$$

It follows from Lemma 9 that the centered Euler scheme is stable for all $\mu \neq 0$. Of course, it is stable at $\mu = 0$. Hence the centered Euler scheme is H-stable.

9.2 H-stability of symplectic invariant methods

Theorem 10. *Symplectic invariant methods are H-stable.*

Proof. By Corolary 6, a symplectic invariant method preserves all quadratic first integrals of linear Hamiltonian systems. For the test Hamiltonian system (9.2), the Hamiltonian itself, $H(z) = \frac{\alpha}{2}z^T z = \frac{\alpha}{2}\|z\|^2$, is a first integral. So $H(z) = \frac{1}{2}\alpha\|z\|^2$ is also a first integral of the symplectic method, i.e., if $z^k, k \geq 0$ is the solution of (9.1) applying to the test system (9.3), then

$$h(z^{k+1}) = h(z^k) = \cdots = h(z^0).$$

Therefore $\|z^k\| = \|z^0\|, k \geq 1$. This means that (9.1) is H-stable.

9.3 H-stability intervals of some explicit symplectic schemes

Explicit symplectic schemes constructed in section 4 are not symplectic invariant. We now consider the H-stability intervals of the 1st–4th order explicit symplectic schemes (4.6), (4.7), (4.11) and (4.8).

Applying the explicit symplectic schemes (4.6), (4.7), (4.11) and (4.8) to the test system (9.3), we get

$$z^{k+1} = G_i(\mu)z^k, \qquad \mu = \alpha s, \quad i = 1, 2, 3, 4, \tag{9.6}$$

respectively, where G_i are their step transition matrices,

$$G_1(\mu) = \begin{pmatrix} 1 & -\mu \\ \mu & 1 - \mu^2 \end{pmatrix},$$

$$G_2(\mu) = \begin{pmatrix} 1 - \frac{1}{2}\mu^2 & -\mu \\ \mu(1 - \frac{1}{4}\mu^2) & 1 - \frac{1}{2}\mu^2 \end{pmatrix},$$

$$G_3(\mu)=\begin{pmatrix} 1-\frac{1}{2}\mu^2+\frac{1}{72}\mu^4 & -\mu(1-\frac{1}{6}\mu^2+\frac{7}{1728}\mu^4) \\ \mu(1-\frac{1}{6}\mu^2+\frac{1}{72}\mu^4) & 1-\frac{1}{2}\mu^2+\frac{5}{72}\mu^4-\frac{7}{1728}\mu^6 \end{pmatrix}.$$

$$G_4(\mu)=\begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix},$$

$$a_1=1-\frac{1}{2}\mu^2+\frac{1}{24}\mu^4+\frac{1}{144}(1+\beta)^2\mu^6,$$

$$a_2=-\mu(1-\frac{1}{6}\mu^2-\frac{1}{216}(2+\beta)(1+2\beta)\mu^4),$$

$$a_3=\mu(1-\frac{1}{6}\mu^2+\frac{1}{216}(2+\beta)(1-\beta)\mu^4+\frac{1}{864}(2+\beta)(1+\beta)^2\mu^6),$$

$$a_4=1-\frac{1}{2}\mu^2+\frac{1}{24}\mu^4+\frac{1}{144}(1+\beta)^2\mu^6.$$

Hence, their H-stability intervals are $(-2,2)$, $(-2,2)$, $(-2.507,2.507)$ and $(-1.573,\ 1.573)$ respectively.

§10 Formal Energy and Non-autonomous Perturbed Energy

10.1 Formal energy

In section 8, we mainly considered the conservation of the quadratic first integrals of Hamiltonian systems by symplectic algorithms and the quadratic first integrals of linear symplectic algorithms. Although the Hamiltonian H is a first integral, according to [29], in general, H can not be conserved by a symplectic algorithm. However, symplectic algorithms can have *formal* energies (Hamiltonians). For more details, refer to [11, 22, 53].

Suppose $H^s(z)=H(s,z)$ is a formal power series in s

$$H^s(z)=H(s,z)=\sum_{i=0}^{\infty}s^iH^{(i)}(z). \tag{10.1}$$

The formal phase flow $e^t_{H^s}$ satisfies

$$\frac{de^t_{H^s}}{dt}=J\nabla H^s\circ e^t_{H^s},\quad e^0_{H^s}=1_{2n}. \tag{10.2}$$

If

$$e^t_{H^s}\big|_{t=s}=g^s_H, \tag{10.3}$$

then $H^s(z)$ is called a *formal* energy of the symplectic algorithm g^s_H. In this case,

$$H^s\circ g^s_H=H^s$$

in the convergent domain of (10.1). Hence, g^s_H formally preserves the formal energy H^s.

In the following, we want to determine H^s from g^s_H. Let the generating function of g^s_H with the normal Darboux matrix α be

$$\phi^t_{H^s,\alpha}(w):=\chi(t,s,w)=\sum_{k=1}^{\infty}t^k\chi^{(k)}(s,w). \tag{10.4}$$

The coefficients $\chi^{(k)}(s,w)$ can be recursively determined

$$\chi^{(1)}(s,w) \quad = \quad -H(s,w),\qquad k\geq 1, \tag{10.5}$$

$$\chi^{(k+1)}(s,w) = -\frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{k_1+\cdots+k_m=k} D_w^m H(a_1\nabla\chi^{(k_1)},\cdots,a_1\nabla\chi^{(k_m)})$$

$$= \frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{k_1+\cdots+k_m=k} D^m\chi^{(1)}(a_1\nabla\chi^{(k_1)},\cdots,a_1\nabla\chi^{(k_m)}), \quad (10.6)$$

where the gradient ∇ is with respect to w. Let

$$\chi^{(k)}(s,w) = \sum_{i=0}^{\infty} s^i \chi^{(k,i)}(w), \quad (10.7)$$

then

$$\chi^{(k+1)}(s,w) = \sum_{i=0}^{\infty} s^i \chi^{(k+1,i)}(w)$$

$$= \sum_{i=0}^{\infty} s^i \frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{i_0+\cdots+i_m=i\\ k_1+\cdots+k_m=k}} D_w^m\chi^{(1,i_0)}(a_1\nabla\chi^{(k_1,i_1)},\cdots,a_1\nabla\chi^{(k_m,i_m)}).$$

Thus

$$\chi^{(k+1,i)}(w) = \frac{1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{i_0+\cdots+i_m=i\\ k_1+\cdots+k_m=k}} D_w^m\chi^{(1,i_0)}(a_1\nabla\chi^{(k_1,i_1)},\cdots,a_1\nabla\chi^{(k_m,i_m)}).$$

So the coefficient $\chi^{(k+1,i)}$ can be recursively determined. From (10.1), (10.5) and (10.7) it follows that

$$\chi^{(1,i)}(w) = -H^{(i)}(w), \quad i = 0,1,2,\cdots. \quad (10.8)$$

Assume that the generating function of g_H^s with the normal Darboux matrix α is

$$\psi_{g,\alpha}(s,w) = \sum_{k=1}^{\infty} s^k \psi^{(k)}(w). \quad (10.9)$$

Condition (10.3) can be rewritten in generating functions as

$$\chi(t,s,w)\Big|_{t=s} = \chi(s,s,w) = \psi(s,w),$$

i.e.,

$$\sum_{k=1}^{\infty} s^k \sum_{i=0}^{\infty} s^i \chi^{(k,i)}(w) = \sum_{k=1}^{\infty} s^k \sum_{i=0}^{k-1} \chi^{(k-i,i)}(w) = \sum_{k=1}^{\infty} s^k \psi^{(k)}(w).$$

It follows

$$\sum_{i=0}^{k-1} \chi^{(k-i,i)}(w) = \psi^{(k)}(w), \quad k = 1,2,\cdots.$$

Therefore,

$$\begin{aligned}
&\chi^{(1,0)} = \psi^{(1)},\\
&\chi^{(1,1)} = \psi^{(2)} - \chi^{(2,0)},\\
&\chi^{(1,2)} = \psi^{(3)} - (\chi^{(3,0)} + \chi^{(2,1)}), \quad (10.10)\\
&\qquad \cdots\cdots\\
&\chi^{(1,k)} = \psi^{(k+1)} - (\chi^{(k+1,0)} + \chi^{(k,1)} + \cdots + \chi^{(2,k-1)}),
\end{aligned}$$

Notice that $\chi^{(k+1,i)}$ can be determined by $\chi^{(k',i')}$, $k' \le k$, $i' \le i$. Then from $\psi^{(i)}$ we can get $\chi^{(1,i)}, i = 0, 1, 2, \cdots$ by (10.10) and hence $H^{(i)}, i = 0, 1, 2, \cdots$ by (10.8) , i.e.,

$$H^{(i)} = -\chi^{(1,i)}, \qquad i = 0, 1, \cdots . \tag{10.11}$$

Finally we get the formal energy

$$H^s = \sum_{i=0}^{\infty} s^i H^{(i)}(z).$$

10.2 Non-autonomous perturbed energy

Formal energy of a symplectic algorithm is a good approximation to the original Hamiltonian. But usually, the convergence of the formal power series can not be guaranteed. There is another kind of non-autonomous perturbed energy of symplectic algorithms which can also exactly reproduce the symplectic algorithm but can not be conserved. For more details, refer to [44].

Since g_H^s is symplectic for all s, i.e.,

$$(g_*^s)^T J g_*^s = J, \qquad \forall s, \tag{10.12}$$

differentiating it with respect to s, we then get

$$\left(\frac{dg_*^s}{ds}\right)^T J g_*^s + (g_*^s)^T J \frac{dg_*^s}{ds} = 0.$$

Therefore

$$J\frac{dg_*^s}{ds}(g_*^s)^{-1} = -(g_*^s)^{-T}\left(\frac{dg_*^s}{ds}\right)^T J = \left(J\frac{dg_*^s}{ds}(g_*^s)^{-1}\right)^T .$$

But

$$J\frac{dg_*^s}{dt}(g_*^s)^{-1} = (J\frac{dg^s}{dt} \circ (g^t)^{-1})_* .$$

This shows that the Jacobian of $J\frac{dg^s}{ds} \circ (g^s)^{-1}$ is symmetric. By Poincare Lemma, there is a function $\overline{H}(\cdot, s) : \mathbf{R}^{2n} \to \mathbf{R}$ such that

$$J\frac{dg^s}{ds} \circ (g^s)^{-1}(z) = \nabla \overline{H}(z, s),$$

i.e.,

$$\frac{dg^s}{ds} = J\nabla \overline{H} \circ g^s .$$

This shows that $\hat{z}(s) = g_H^s(z)$ is the solution of the non-autonomous Hamiltonian system

$$\frac{dz}{ds} = J\nabla \overline{H}(z, s).$$

More precisely,

$$\overline{H}(z, s) = \int_0^1 z^T J \frac{dg^s}{ds} \circ (g^s)^{-1}(\alpha z)\, d\alpha .$$

It follows that

$$\overline{H}(z, s) = H(z) + O(s^r).$$

Example 1. For the linear symplectic algorithm (8.15), the corresponding time dependent Hamiltonian is

$$\overline{H}(z, s) = \frac{1}{2} z^T J \frac{dG(s)}{ds} G^{-1}(s) z,$$

which is different from (8.18)

Example 2. For the seperable Hamiltonian

$$H(p,q) = U(p) + V(q), \qquad p, q \in \mathbf{R}^n,$$

a first order explicit symplectic difference scheme is

$$g^s: \qquad \hat{p} = p - sV_q(q), \quad \hat{q} = q + sU_p(\hat{p}).$$

The perturbed Hamiltonian is

$$\overline{H}(p,q,s) = U(p) + V(q - sU_p(p)).$$

A second order explicit symplectic difference scheme is

$$g^s: \qquad q^* = q + \frac{s}{2}U_p(p), \quad \hat{p} = p - sV_q(q^*), \quad \hat{q} = q^* + \frac{s}{2}U_p(\hat{p}).$$

The perturbed Hamiltonian is

$$\overline{H}(p,q,s) = \frac{1}{2}U(p) + \frac{1}{2}U(p + sV_q(q - \frac{s}{2}U_p(p)) + V(q - \frac{s}{2}U_p(p)).$$

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