Hichael Nices

Thorough of of

The next !

The A.

SYMPLECTIC INTEGRATORS

Michael K. Pierce

May 23, 1994

1 Introduction

The goal of this paper is to give a brief introduction to symplectic integrators as well as describe some interesting results. It relies primarily upon the results of 5 main papers [4],[5],[6],[8] and [9], in an attempt to give a background for ongoing research in this area.

2 Symplectic Difference Schemes

2.1 What Are They?

Definition: A symplectic difference scheme is a rule which assigns to every Hamiltonian function H(z) a symplectic map D_H^{τ} depending smoothly on a parameter τ .

 D_H^{τ} needs to approximate the solution of a Hamiltonian system $\frac{d}{dt}(z) = J^{-1}dH(z)$, so we require

$$\frac{D_H^{\tau}(z) - D_H^0(z)}{t} = J^{-1}dH(z) + O(z). \tag{1}$$

For instance, the midpoint rule

$$z^{k+1} = z^k + \tau J^{-1} dH(\frac{z^{k+1} + z^k}{2})$$
 (2)

is a first order symplectic difference scheme, which approximates the flow of a Hamiltonian system.

Testing whether or not a difference scheme is symplectic is usually a straightforward calculation on the canonical symplectic structure. If (q,p) are canonical symplectic coordinates, and $D_H^{\tau}(q,p)=(\bar{q},\bar{p})$, just show $dq \wedge dp=d\bar{q} \wedge d\bar{p}$. The order of a symplectic scheme will not be discussed in this paper, but there are ways to obtain higher order symplectic schemes from first order ones.

2.2 Creating Symplectic Difference Schemes by Generating Functions

Determining whether a scheme is symplectic or not can be a straightforward calculation, but constructing a symplectic sceme which approximates the flow can be much harder. One technique for constructing such schemes is by use of generating functions. The basic idea is to find a generating function which approximates the solution of a time dependent Hamilton-Jacobi equation and use this function to generate a symplectic map which approximates the flow of the Hamiltonian system.

The main fact used in finding a generating function is that the graph of a symplectic transformation is a Lagrangian submanifold of the product space. Choosing symplectic coordinates (q,p) on our space, let $S(q,p)=(\bar{q},\bar{p})$ be a symplectic transformation. Look at the graph of this map $gra(S)=\{((\bar{q},\bar{p}),(q,p)):S(q,p)=(\bar{q},\bar{p})\}$. Then by definition $d\bar{q} \wedge d\bar{p} - dq \wedge dp = 0$ on gra(S). In other words, gra(S) is a Lagrangian submanifold in (R^{4n},ω_1) where $\omega_1 = d\bar{q} \wedge d\bar{p} - dq \wedge dp$. In addition, R^{4n} has a standard symplectic structure ω_2 with symplectic coordinates (w,\bar{w}) , $\omega_2 = dw \wedge d\bar{w}$. Moreover, a submanifold which is locally Lagrangian in (R^{4n},ω_2) can be written locally as $\{(w,\bar{w}): \bar{w} = \frac{\partial U}{\partial w}\}$ for some function U.

Definition: A generating map is a linear transformation $\Phi: R^{4n} \longrightarrow R^{4n}$, for which $\Phi^*\omega_2 = \omega_1$. In particular, Φ maps Lagrangian submanifolds of (R^{4n}, ω_1) to Lagrangian submanifolds of (R^{4n}, ω_2) .

Therefore, Φ maps gra(S) to a Lagrangian submanifold of (R^{4n}, ω_2) which can locally be given in terms of some function U. This U is called the generating function corresponding to the generating map Φ . Different generating maps Φ will give rise to different generating functions U, which will determine different symlectic transformations S.

Example 1. Let Φ be given by

$$\Phi = \begin{bmatrix} -J_{2n} & J_{2n} \\ \frac{J_{2n}}{2} & \frac{J_{2n}}{2} \end{bmatrix} \tag{3}$$

$$\Phi(\bar{p},\bar{q},p,q)=(\bar{w},w).$$

Then U gives rise to the symplectic transformation S is defined by

$$\bar{z} - z = -J \frac{\partial U}{\partial w} (\frac{\bar{z} + z}{2}). \tag{4}$$

This is called Poincare's generating function.

Example 2. Another type is given by

$$\Phi = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & I_n & 0 \\ 0 & I_n & 0 & 0 \\ 0 & 0 & 0 & I_n \end{bmatrix}.$$
 (5)

Where U gives rise to the map S defined by

$$\bar{p} = -\frac{\partial U}{\partial \bar{q}}(\bar{q}, q), p = \frac{\partial U}{\partial q}(\bar{q}, q). \tag{6}$$

This is known as a generating funcion of the first type. •

For a general generating map Φ , suppose $U_{\phi}(w,t)$ is the generating function for the phase flow ϕ_t of the Hamiltonian function H. Then U_{ϕ} satisfies the Hamilton-Jacobi equation

$$\frac{\partial U_{\phi}}{\partial t} = H \circ pr_2 \circ \Phi^{-1}(w, \frac{\partial U_{\phi}}{\partial w}). \tag{7}$$

Where pr_2 is the map $(\bar{z}, z) \longrightarrow z$. So to get our symplectic scheme, find an approximate solution \mathcal{U} to (7) and solve $\bar{w} = \frac{\partial \mathcal{U}}{\partial w}$.

2.3 Example

The following is an example of the above process for the construction of a symplectic integrator to approximate a solution to the Henon-Heiles equations

$$\frac{d}{dt} \begin{bmatrix} p_1 \\ p_2 \\ q_1 \\ q_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} p_1 \\ p_2 \\ q_1 + 2q_1q_2 \\ q_2 + q_1^2 - q_2^2 \end{bmatrix}$$
(8)

based upon an example in [4]. The above equations determine a Hamiltonian system with Hamiltonian

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2 + 2q_1^2q_2 - \frac{2}{3}q_2^3).$$

To construct an integrator, first choose our generating map to be

$$\Phi = \begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_n \\ 0 & I_n & 0 & 0 \\ 0 & 0 & I_n & 0 \end{bmatrix}$$
(9)

which is known as a generating map of the second kind. If M is our symplectic manifold, with canonical coordinates (q, p), and S is our symplectic map such that $S(q, p) = (\bar{q}, \bar{p})$, then this map Φ determines

$$w = (\bar{q}, p), \bar{w} = (-\bar{p}, -q) = (\frac{\partial U}{\partial \bar{q}}, \frac{\partial U}{\partial p}),$$

with $U(\bar{q}, p, t)$ the corresponding generating function. This leads to the Hamilton-Jacobi equation

$$\frac{\partial U}{\partial t} = -H(p, -\frac{\partial U}{\partial p}).$$

Approximate the solution by the first order taylor's series expansion with respect to time to get

$$\mathcal{U}(\bar{q},p)=U_0(\bar{q},p)+U_1(\bar{q},p)\tau.$$

Let $U_0(\bar{q}, p) = -\bar{q}p$, and from above $U_1(\bar{q}, p) = -H(p, q)$. So

$$\mathcal{U}(\bar{q},p) = -\bar{q}p - \tau H(p,q)$$

and

$$\bar{w} = \frac{d\mathcal{U}}{dw} = \begin{bmatrix} p - \tau H_q(p, q) \\ \bar{q} - \tau H_p(p, q) \end{bmatrix} = \begin{bmatrix} -\bar{p} \\ -q \end{bmatrix}$$

leads to the difference scheme

$$p_1^{n+1} = p_1^n - \tau(q_1^n + 2q_1^n q_2^n)$$

$$p_2^{n+1} = p_2^n - \tau(q_2^n + (q_1^n)^2 - (q_2^n)^2)$$

$$q_1^{n+1} = q_1^n + \tau p_1^{n+1}$$

$$q_2^{n+1} = q_2^n + \tau p_2^{n+1}.$$
(10)

The figures at the end compare this symplectic difference scheme (10) to a Runge-Kutta second order method. The first figure shows the error of the two methods in computing a solution curve with respect to the solution of a Runge-Kutta method of order 4. The second figure shows the values of the Hamiltonian under successive time steps.

From the first figure, it appears that RK2 might be a better method to run than our symplectic scheme because the error tends to be a little less. But, the second figure shows the symplectic method tends to preserve the Hamiltonian better on average. Since it is expected that our actual solution has constant Hamiltonian, the symplectic method is more accurate when integrating over long time intervals. This even puts to question whether to use the second order symplectic method instead of RK4 itself.

3 Constrained Symplectic Difference Schemes

The previous section showed examples of how to create symplectic schemes on \mathbb{R}^n . The present section takes our created symplectic scheme and restricts it to a submanifold. As seen by example [9], the new scheme may or may not be symplectic on the new space.

Let a Hamiltonian system be given on a symplectic manifold M constrain the dynamics to a submanifold $N \subset M$. Suppose a function $\phi: M \longrightarrow V$ is given, where V is a linear space, such that $N = \{x \in M : \phi(x) = 0\}$. We want to construct an integrator $S: N \longrightarrow N$ which approximates the constrained dynamics on N.

Example: Shake and Rattle

As an example of constaining a symplectic difference scheme we look an the Shake and Rattle schemes given in [9]. Consider a system of vibrating molecules which lead to the Hamiltonian system of the form

$$M\dot{q} = p$$

$$\dot{p} = -\nabla_{q} V(q). \tag{11}$$

Constrain the system to a submanifold N by fixing some bond lengths and angles,

$$N = \{(q, p) : g(q) = 0, g'(q)M^{-1}p = 0\}.$$
(12)

This leads to the new system

$$M\dot{q} = p$$

$$\dot{p} = -\nabla_q V(q) + g'(q)^{\mathsf{T}} \lambda$$

$$g(p) = 0.$$
(13)

The Hamiltonian equations (11) can be approximated by a symplectic difference scheme similar to those defined above. One such method is known as the Verlet scheme

$$q_{n+1} = q_n + h M^{-1} p_{n+\frac{1}{2}}$$

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2} \nabla_q V(q_n)$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} \nabla_q V(q_{n+1})$$
(14)

where h is the time stepsize.

This symplectic difference scheme can be adapted to one on the constrained system (13) in different ways. One "constrained" method known as the Shake algorithm is given by:

$$q_{n+1} = q_n + h p_{n+\frac{1}{2}}$$

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2} \nabla_q V(q_n) + \frac{h}{2} g'(q_n)^{\mathsf{T}} \lambda_n$$

$$g(q_{n+1}) = 0 \tag{15}$$

$$p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} \nabla_q V(q_{n+1}) + \frac{h}{2} g'(q_{n+1})^{\mathsf{T}} \lambda_{n+1}$$

where we assume M = I. This method is not a symplectic method on N because although $g(q_n) = 0$ at every point, we do not generally have $g'(q_n)M^{-1}p_n = 0$, even if we start on N. But looking at (15) as a method on $N_0 = \{(q, p) : g(p) = 0\}$, (15) does preserve the symplectic form on this new manifold. So (15) is a symplectic difference scheme on N_0 .

The Rattle method is a correction to the Shake method. The Rattle method projects the momenta p_{n+1} of the Shake method onto the manifold N. This makes the Rattle method map from N to N symplecticly. It is given by

$$q_{n+1} = q_n + h p_{n+\frac{1}{2}}$$

$$p_{n+\frac{1}{2}} = p_n - \frac{h}{2} \nabla_q V(q_n) + \frac{h}{2} g'(q_n)^{\mathsf{T}} \lambda_n$$

$$g(q_{n+1}) = 0 \tag{16}$$

$$p_{n+1} = (I - \mathcal{H}(q_{n+1}))(p_{n+\frac{1}{1}} - \frac{h}{2} \nabla_q V(q_{n+1}) + \frac{h}{2} g'(q_{n+1})^{\mathsf{T}} \lambda_{n+1})$$

where $\mathcal{H}(q) = g'(q)^{\mathsf{T}}(g'(q)g'(q)^{\mathsf{T}})^{-1}g'(q)$ is the projector matrix.

Although this method is symplectic and preserves the submanifold N, it may not be the best algorithm to use in general. The Shake scheme is still symplectic on N_0 and is easier to implement than the Rattle scheme. According to [9], if the constraint relationships are solved accurately enough, the Shake and Rattle schemes give equivalent results. Therefore it would be ideal to use a sequence of Shake scheme steps followed by one Rattle scheme step.

4 Invariance

In addition to preserving the symplectic structure, difference schemes may also conserve other quantities of the Hamiltonian system. This section examines some quantities a symplectic difference scheme may conserve and how to construct them.

4.1 Invariance of Difference Schemes Under Phase Flow

Definition: A symplectic difference scheme D_H^{τ} is invariant under symplectic coordinate transformation T if $T^{-1} \circ D_H^{\tau} \circ T(w) = D_{T \circ H}(w)$.

Example 1. The midpoint difference scheme is given by the formula

$$\frac{z^{k+1} - z^k}{\tau} = J^{-1}dH(\frac{z^{k+1} + z^k}{2}). \tag{17}$$

Suppose T is a symplectic coordinate transformation such that T(w) = z for another coordinate w. Then the midpoint scheme on w takes the form

$$\frac{w^{k+1} - w^k}{\tau} = J^{-1}dH(T(\frac{w^{k+1} + w^k}{2}))$$
 (18)

because the function H now has the form $H \circ T$. Rewriting (17) in terms of w coordinates, implies

$$\frac{T(w^{k+1}) - T(w^k)}{\tau} = J^{-1}dH(\frac{T(w^{k+1}) + T(w^k)}{2}). \tag{19}$$

For general symplectic coordinate tranformation T, the right hand sides of (18) and (19) are not equal, so lead to different difference schemes. If we assume that T is linear, then (19) becomes

$$\frac{T(w^{k+1} - w^k)}{\tau} = J^{-1}dH(T(\frac{w^{k+1} + w^k}{2}))$$
 (20)

$$JT(\frac{w^{k+1} - w^k}{\tau}) = dH(T(\frac{w^{k+1} + w^k}{2})). \tag{21}$$

Since the midpoint scheme is invariant under the linear symplectic transformation group, and since the quadratic functions generate a one-parameter group of linear symplectic transformations [6], by the theorem proved next, the midpoint scheme preserves quadratic first integrals.

Theorem 1. A symplectic difference scheme D_H^{τ} preserves a first integral f of H up to a constant

$$f \circ D_H^\tau = f + c$$

if and only if the scheme D_H^{τ} is invariant under the phase flow of f.

proof: [6].□

The next question to ask is whether or not a symplectic difference schemes can be created which preserve all the first integrals of a Hamililtonian H. Supposedly this would give us best approximation to our system of all. The answer is no.

Theorem 2: Assume H has no other first integrals besides itself. If D_H^{τ} is a symplectic difference scheme which preserves H exactly, then it is the exact solution for the Hamiltonian system up to a reparametrization of time.

proof: D_H^{τ} was defined earlier as being a one-parameter symplectic map depending smootly on the parameter τ , with $D_H^0 = Id$. Let $F(z,\tau)$ be the Hamiltonian function for this one-parameter family of symplectic transformations. Because $H \circ D_H^{\tau} = H$, we have $\{F, H\} = 0$, ie. F is a first integral for fixed τ . So $F(z,\tau) = F_1(H(z),\tau)$ for some F_1 because we already said H is the only first integral. Now look at the Hamiltonian vector field of $F(z,\tau)$,

$$J^{-1}dF(z,\tau) = J^{-1}d(F_1(H(z),\tau)) = J^{-1}dF_1(H(z),\tau) \circ dH(z). \tag{22}$$

On a level set H(z) = h, this becomes

$$= J^{-1}dF_1(h,\tau) \circ dH(z), \tag{23}$$

which is just multiplication by a scalar depending on τ . Therefore, the vector fields generated by F and H differ oly by a scalar multiple of τ . Hence the phase flow of F restricted to H = h differs from that of H by a reparametrization of time. \square

Now if our Hamiltonian system has other first integrals besides H, we can reduce our space by the one-parameter groups generated by the first integrals and end up with a difference scheme on the reduced space. If this scheme is symplectic then it contradicts Theorem 2 because the only first integral left is H.

4.2 Invariance of Generating Functions

Definition: For a fixed generating map Φ , a generating function is invariant under T if there is a transformation $A: R^{4n} \longrightarrow R^{4n}$ independent of ϕ_{τ} such that for local symplectic transformation ϕ_{τ}

$$U_{T^{-1}\circ\phi_{\tau}\circ T}=U_{\phi_{\tau}}\circ A.$$

where U_{Ψ} is the generating function for the symplectic map Ψ and T is a symplectic coordinate transformation.

Example 1. Poincare's generating function is invariant under any linear symplectic transformation [6].

Now using Theorem 1 from above, we get the following result.

Corollary 1: Suppose H has a first integral f, and that the generating function is invariant under the phase flow of f. Then the symplectic difference scheme constructed by this generating function preserves f up to a constant.

proof: This follows directly from Theorem 1 if it can be shown that if T is a symplectic map under which the generating function is invariant, then the difference scheme for H, constructed by this generating function, is invariant under T. Suppose the generating function is invariant under T. Then

$$U_{T^{-1}\circ\phi_H^{\mathfrak{t}}\circ T}=U_{\phi_H^{\mathfrak{t}}}\circ A$$

for some A by definition. Where ϕ_H^t is the Hamiltonian flow for H. Since ϕ_H^t is the flow of the Hamiltonian H, let $\phi_{H\circ T}^t$ be the flow of $H\circ T$, then

$$T^{-1} \circ \phi_H^t \circ T = \phi_{H \circ T}^t.$$

Hence

$$U_{\phi_{H \circ T}^{\mathfrak{t}}} = U_{\phi_{H}^{\mathfrak{t}}} \circ A$$

Expanding both sides to its taylor series expansion, we see

$$\frac{d^{i}}{dt^{i}}\mid_{t=0} U_{\phi_{H \circ T}^{i}} = \frac{d^{i}}{dt_{i}}\mid_{t=0} U_{\phi_{H}^{i}} \circ A.$$

So

$$\frac{d^i}{dt^i}\mid_{t=0} U_{\phi^i_{H \circ T}} = \frac{d^i}{dt^i}\mid_{t=0} U_{T^{-1} \circ \phi^i_{H} \circ T}$$

by invariance of the generating function. So approximating up to k terms to get the difference scheme

$$D^\tau_{H \circ T} = T^{-1} \circ D^\tau_H \circ T$$

This theorem gives us a more general idea of how to construct symplectic difference schemes which preserve the desired quantities. In theory, pick an approximation to our Hamilton-Jacobi equation which is invariant under the phase flow of f, then the difference scheme will automatically conserve f.

5 Symplectic Difference Schemes on T^*M

Now examine our results above on a special type of symplectic space, T^*M . Let T^*M have the canonical symplectic structure $\omega = dq \wedge dp$ and take $\Phi: T^*M \times T * M \longrightarrow T^*(M \times M)$, $\Phi(\bar{p}, \bar{q}, p, q) = (-\bar{p}, p, \bar{q}, q)$ as the generating map. This is a globalization of the first type of generating map. Identify $T_q^*M \times T_{\bar{q}}^*M$ with $T_{(q,\bar{q})}^*(M \times M)$ and let $S: T^*M \longrightarrow T^*M$ be a symplectic transformation. So now Φ maps gra(S) to a Lagrangian submanifold L in $T^*(M \times M)$.

Definition: Suppose L satisfies the following condition at (q_0, p_0) : The projection $pr: (-\bar{p}, p, \bar{q}, q) \longrightarrow (\bar{q}, q) \in M \times M$ is a local diffeomorphism at (\bar{p}_0, q_0) where $S(p_0, q_0) = (\bar{p}_0, \bar{q}_0)$. Then S is called free at (p_0, q_0) .

Locally, L can be written as $\{(\frac{\partial U}{\partial \bar{q}}, \frac{\partial U}{\partial q}, \bar{q}, q)\}$, for a local funcion U on $M \times M$, hence S can be defined locally by $\bar{p} = \frac{\partial U}{\partial \bar{q}}$, $p = \frac{\partial U}{\partial q}$. Now suppose the group G acts on M and hence symplectically on T^*M . Then we have the momentum map defined by $\langle J(p,q), \xi \rangle = (p, \xi_{T^*M}(q))$, which is equivariant. Then by [], leads to

Proposition 1. Suppose S is a symplectic tranformation preserving J and free at (p_0, q_0) , then the generating function U_S can be defined on an open set in $M \times M$ containing (\bar{q}_0, q_0) and invariant under the induced action on G on $M \times M$.

proof: [6].□

corollary 2. Symplectic difference schemes constructed via the first type of generating function preserve the momentum J.

proof: This follows from proposition 1 and corollary 1.□

6 Lie-Poisson Difference Schemes

The goal of this section is to outline the process of reducing a symplectic difference scheme on a special symplectic manifold T^*G to a scheme on $T^*G/G \cong \mathcal{G}^*$. Assume a generating function U of the first type exists, and that U and Hamiltonian H are invariant under the group action. The idea is to reduce the generating function U to a generating function on \mathcal{G}^* . To do this, the Hamilton-Jacobi equations on T^*G are reduced to equations on \mathcal{G}^* .

Proposition 2. If U is group invariant, there is a unique function U_L such that $U(g,g_0)=U_L(g^{-1}g_0)$, and the left reduced Hamilton-Jacobi equation is the following equation for the function $U_L: G \longrightarrow R$.

$$\frac{\partial U_L}{\partial t} + H_L(-TR_g^* \circ dU_L(g)) = 0$$

where H_L is the left reduced Hamiltonian on \mathcal{G}^{-} . proof: [8]. \square

The flow of H_L on \mathcal{G}^* is then given by the poisson transformation generated by S_L , defined as follows:

Define $g \in G$ by solving $\Pi_0 = -TL_g^* \circ d_g U_L$. Then set $\Pi = Ad_{g^{-1}\Pi_0}^*$. So the transformation is $\Pi_0 \longrightarrow \Pi$, ie. $\Pi = Ad_{g^{-1}}^* (-TL_g^* d_g U_L)$. Another way to look at this is that on T^*G we have

$$J_L(q,p) = R_q^*(p), J_R(q,p) = L^*q(p).$$

Then a poisson tranformation $\phi_0(z) = \bar{z}$ on \mathcal{G}^* generated by a generating function U is given by

$$\phi_L(z) = \bar{z}, J_L(q, \frac{\partial U_L}{\partial q}) = z, J_R(q, \frac{\partial U_L}{\partial q}) = \bar{z}.$$
 (24)

Let $S: T^*G \longrightarrow T^*G$ be a symplectic map preserving J_L , given by a generating function U. Then by Corollary 1, U is invariant under the action of G on $G \times G$, and from earlier $U = U_L(q, \bar{q}^{-1})$. Therefore S can be reduced to $S_L: \mathcal{G}^* \longrightarrow \mathcal{G}^*$, by letting $S_L(p) = J_R \circ S(e, p)$. And so can be given by (?).

Ge-Marsden give a general way to construct first order Lie-Poisson integrators. Let $H: \mathcal{G}^* \longrightarrow R$ be a Hamiltonian function and let U_0 be a function which generates a poisson transformation $\phi_0: \mathcal{G}^* \longrightarrow \mathcal{G}^*$. Let $U_{\Delta t} = U_0 + \Delta t H(L_g^* dU_0)$. For small t, this generates a poisson transformation $\phi_{\Delta t}: \mathcal{G}^* \longrightarrow \mathcal{G}^*$.

Proposition 3. The algorithm $\Pi^k \longrightarrow \Pi^{k+1} = \phi_0^{-1} \circ \phi_{\triangle t}(\Pi^k)$ is a first order poisson difference scheme for the Hamiltonian system with Hamiltonian H.

7 Hamilton-Poisson Generalization

In [5] Ge Zhong describes a way to generalize the construction of Lie-Poisson integrators to spaces which are just Poisson. Such systems may arise when infinite dimensional systems are descretized to finite dimensional ones.

The Lie-Poisson case depended upon generating functions in order to create our symplectic difference scheme, which is then reduced to \mathcal{G}^{\bullet} . So we first need to define a notion for generating function on a general Poisson manifold P.

Definition: A pair (S, J) is a generating pair for a Poisson manifold P if:

- 1. S is a symplectic manifold, J is a Poisson map from S to $P \times P^-$, $J: S \longrightarrow P \times P^-$ (P^- is the same manifold as P with the poisson bracket multiplied by -1).
- 2. J maps local Lagrangian submanifolds in S to the graphs of local Poisson automorphisms of P.

And is a strict generating pair if it satisfies the extra condition

3. There is a Lagrangian submanifold L_0 such that J maps L_0 diffeomorphically to the graph of the identity automorphism of P.

Definition: If we have a generating pair (S, J), $J: S \longrightarrow P \times P^-$, then adopting local canonical coordinates (q, p) on S, a Lagrangian submanifold L can be given by a generating function U

$$L = \{(q, \frac{\partial U}{\partial q})\}$$

and the Poisson transformation $A: P \longrightarrow P$ whose graph is J(L) can be written in terms of U as

$$A(z) = \bar{z}, z = J_1(q, \frac{\partial U}{\partial q}), \bar{z} = J_2(q, \frac{\partial U}{\partial q}).$$

U is the generating function of the Poisson transformation A.

Example 1. $(T^*G, J = J_L \times J_R)$ is a generating pair

$$J=J_L\times J_R:T^*G\longrightarrow \mathcal{G}^*\times \mathcal{G}^*_-$$

where J_L , J_R are the momentum maps for the left and right actions of G. Then a generating funtion U on G gives rise to a Poisson transformation

$$A(z) = \bar{z}, z = R_a^* dU, \bar{z} = L_a^* dU$$

Theorem 3. Suppose (S, J) is a generating pair. If U(q, t) are the generating functions for the Lagrangian submanifolds $L^t = \{(q, dU(q, t))\}$, such that the images

 $J(L^t) \in P \times P^-$ are the graphs of the phase flow of the Hamilton-Poisson system $\dot{F} = \{F, H\}$, then U(q, t) satisfies the Hamilton-Jacobi equation

$$\dot{U}_t = H \circ J_1(q, dU).$$

So in the same manner as for the symplectic case, we can construct Poisson transformations if there exists a generating function, or in this case a generating pair. To understand when generating pairs exist, we need to look at a few more results in [5].

Definition: A realization of a Poisson manifold P is a Poisson map from a symplectic manifold S to P,

$$J: S \longrightarrow P$$
.

If a realization J is a submersion, then we say it is a full realization.

Definition: A full dual pair is two full realizations

$$J_1: S \longrightarrow P, J_2: S \longrightarrow P^-$$

provided that $kerTJ_1$, $kerTJ_2$ are symplectic orthogonal complements of each other.

Theorem 4. Suppose that (S, P, J_1, J_2) is a full dual pair, then $J_1 \times J_2 : S \longrightarrow P \times P^-$ maps every Lagrangian submanifold L intersecting the level surfaces $J_1 = constant$, $J_2 = constant$ transversely to the graph of a (local) Poisson transformation of P.

Theorem 5. Suppose that J_1 , J_2 are full realizations of P, P^- respectively,

$$J_1: S \longrightarrow P, J_2: S \longrightarrow P^-:$$

then (S, J), where $J = J_1 \times J_2$ is a generating pair if and only if J_1 , J_2 is a dual pair.

So the construction of Poisson integrators by generating functions will depend on the existence of dual pairs. The proofs are omitted because they require a framework too lengthy to be included here, but can be found in [5].

8 References

- [1] P.J. Channell and C. Scovel, Symplectic Integration on Hamiltonian Systems, Non-linearity 3 (1990), 231-59.
- [2] P.J. Channell and C. Scovel, Integrators for Lie-Poisson Dynamical Systems, Physica D 50, (1990), 80-8.
- [3] K. Feng and Z. Ge, On the approximation of Linear Hamiltonian Sysems, J. of Comp. Math. 6 (1988), 87-97.
- [4] K. Feng and M. Qin, The Symplectic Methods for the Computation of Hamiltonian Equations, in: Numerical Methods for Partial Differential Equations, Proceedings, eds. Zhu You-Ian and Guo Ben-Yu, Lecture Notes in Mathematics, Vol. 1297 (Springer, Berlin, 1988).
- [5] Z. Ge, Generating Functions, Hamilton-Jacobi Equations and Symplectic Groupoids on Poisson Manifolds, Indiana Math. J. 39, (1990), 859-76.
- [6] Z. Ge, Equivariant Symplectic Difference Schemes and Generating Functions, Physica D 49 (1991), 376-86.
 - [7] Z. Ge, Symplectic Integrators for Hamiltonian Systems, (preprint).
- [8] Z. Ge and J.E. Marsden, Lie-Poisson Hamilton-Jacobi Theory and Lie-Poisson Integrators, Phys. Lett. A 133 (1988), 134-9.
- [9] B.J. Leimkuhler and R.D. Skeel, Symplectic Numerical Integrators in Constrained Hamiltonian Systems, (preprint).
- [10] R.I. McLachlan and P. Atela, The Accuracy of Symplectic Integrators, Non-linearity 5 (1992), 541-62.
- [11] R.I. McLachlan and C. Scovel, Equivariant constrained Symplectic Integration, (preprint).
- [12] R.I. McLachlan and C. Scovel, A Survey of Open Problems in Symplectic Integration, (preprint).

- [13] J.M. Sanz-Serna, Symplectic Integrators for Hamiltonian Problems: an Overview, Acta Numerica (1991), 243-86.
- [14] C. Scovel, Symplectic Numerical Integration of Hamiltonian Systems, in: The Geometry of Hamiltonian Systems, ed. Tudor Ratiu, MSRI Publ. 22 (Springer-Verlag, New York, 1991), 463-96.
- [15] J.C. Simo, N. Tarnow and K.K. Wong, Exact Energy-Momentum Conserving Algorithms and Symplectic Schemes for Nonlinear Dynamics, (preprint).
- [16] A. Weinstein, Symplectic Groupoids and Poisson Manifolds, Bull. Amer. Math. Soc. 16 (1987) 101-4.
- [17] A. Weinstein, Coisotropic Calculus on Poisson Groupoids, J. Math. Soc. Japan 40 (1988), 705-27.



