Global Theory of Extended Generating Functions

Bela Erdelyi
Department of Physics, Northern Illinois University,
DeKalb, IL, 60115,
and Physics Division, Argonne National Laboratory,
Argonne, IL, 60439

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Abstract

The global theory of generating functions of canonical transformations is developed. Utilizing methods of symplectic geometry, we present the geometrical interpretation of the various objects appearing in the theory, that allows to define infinitely many types of generators, some of which can be defined globally. Some interesting transformation properties are derived. Use of generators in applications in applied mathematics (symplectic numerical integration) and physics (nonlinear beam dynamics) are outlined.

1 Introduction

Generating functions of canonical transformations are ubiquitous in classical mechanics [1]. Their use ranges from solving analytically mechanical systems to perturbation methods. More recently, generating functions have been used in geometrical integration, namely symplectic numerical integration [2]. Also, a related topic is the so-called symplectification of maps, that is the symplectic approximation of the truncated Taylor series approximation of Hamiltonian symplectic maps [3]. Our interest in extending the theory of generating functions, with an eye to their use in numerical calculations, arose from trying to formulate an optimal theory of symplectification [4]. This theory of optimal symplectification allows fast and accurate simulation of the long-term nonlinear dynamics of Hamiltonian systems, especially of charged particles in particle accelerators. It was realized that the most general way in applying the generating function theory to Hamiltonian dynamical systems is to transform the problem into a problem in symplectic geometry, solve the problem there, and apply back the results in applied mathematics and physics. Since the main motivation came from studying the nonlinear charged particle beam dynamics in accelerators, which are weakly nonlinear Hamiltonian systems, locally around fixed points, a local theory of generating functions has been developed in [5]. In this paper we develop the global theory of extended generating functions using geometrical methods, and in the process we answer some questions left unanswered in the local theory. The use of the generating functions in numerical calculations is outlined.

In the standard literature, traditionally only the 4 Goldstein type of generating functions are well known [1]. However, it is easy to show that, for example, the identity transformation cannot be generated by the type 1 and 4 generating functions. On the other hand, this set can be easily extended to 2^n, or 4^n, generating functions. It can be showed that for any symplectic map, at least one generating function from this set exists locally [6]. The common factor for this set is that they all depend on mixed coordinates, more specifically on n initial coordinates and momenta, and n final coordinates and momenta. The first sign that in fact there are even more generating function types dates back to Poincaré, who used a different type of generating function, which not only is a mixed variable function in the sense discussed above, but also mixes (linearly) initial and final conditions in all the $2n$ variables [7]. Later this generating function reappeared in the symplectic geometry literature [8] and numerical integration literature [9], where also a unifying approach to the theory of generating functions has been presented, from which it resulted that there are infinitely many generating functions. In the following sections we will show in what sense a function generates a canonical transformation locally and globally, what is the freedom in choosing types of generators, how to compute them, and how they transform under various operations on the symplectic maps and the different types of generators. We conclude with a brief summary.

2 The Global Theory

The local theory developed in [5] is sufficient for weakly nonlinear Hamiltonian systems. However, in the general case there are important aspects that the local theory does not answer. For example, how can the theory be extended to symplectic manifolds? Is there a geometric interpretation of the generating function? Is there a more general definition that provides even more generator types than those provided by the local theory? Finally, what can be said about the domain of definition of the generators? Can a global generating function be defined for any symplectic map? In this section we answer these questions.

The local theory shows that around any point local generators can be found. The question is whether the various local generators can be glued smoothly to form a global generator. However, the existence of the appropriate nonlinear conformal symplectic maps is not a priori obvious. Moreover, even if a global generator exists for a given symplectic map, does the same type of generator exist globally for other symplectic maps? The solution of these questions requires the "geometrization" of the problem, that is, reformulation of the problem into a problem in symplectic geometry. We begin with a brief introduction to symplectic geometry, more details can be found in [10, 11].

2.1 Fundamentals of Symplectic Geometry

Symplectic geometry is the natural mathematical language of classical mechanics, specifically Hamiltonian dynamics, as any variational principle can be given a symplectic interpretation. To begin, some fundamental concepts are introduced. Let P be a smooth manifold, and ω a differential 2-form defined on it. If ω is closed and non-degenerate, it is called a symplectic form, and the pair (P, ω) is called a symplectic manifold. A form is called closed if its exterior differential vanishes, $d\omega = 0$. Closedness is a geometric constraint, which is equivalent to the Jacobi identity. On the other hand, non-degeneracy is an algebraic condition. It means that at each point $p \in P$ the skew-symmetric bilinear form $\omega_p : T_pP \times T_pP \to \mathbb{R}$ which acts on tangent vectors, is non-degenerate. In terms of the associated linear map $\tilde{\omega}_p\left(v\right)\left(u\right) = \omega_p\left(v, u\right)$, we have that, if $\tilde{\omega}_p\left(v\right)\left(u\right) = 0$ for each $v \in T_pP$, then $u = 0$. Hence $\tilde{\omega}_p : T_pP \to T_p^*P$ is an isomorphism. This means that, relative to some local coordinate system around each point, the matrix of $\tilde{\omega}$, and equivalently the matrix of ω has nonzero determinant. This in turn implies that any symplectic manifold is necessarily even dimensional, due to the fact that the determinant of any odd dimensional skew-symmetric matrix vanishes.

A fundamental category of symplectic manifolds are the cotangent bundles of configuration manifolds, which are the phase spaces of dynamical systems. These manifolds carry a symplectic structure that is a generalization of the canonical symplectic structure of $\mathbb{R}^{2n}$. On the Euclidean space itself, by identifying $\mathbb{R}^{2n}$ with $T^*\mathbb{R}^n$, we have a special coordinate system in which the symplectic form takes the simple form $\omega_0 = d\vec{q} \wedge d\vec{p}$. The coordinates $(\vec{q}, \vec{p})$ are called canonical. This coordinate system is the symplectic counterpart of the orthonormal coordinate system of Euclidean geometry. The matrix of ω_0 is denoted by J and has the form

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{1}$$

where each entry represents a $n \times n$ block matrix, I being the appropriate unit matrix. We also note that the standard symplectic form can be defined in a coordinate-free way by $\omega_0 = -d\lambda$, where λ is called the canonical one-form, and takes the coordinate representation $\lambda = \vec{p} \cdot d\vec{q}$. Darboux's theorem states that on any symplectic manifold such a coordinate system can be found in a neighborhood of any point, hence any symplectic manifold is locally equivalent (symplectomorphic) to the Euclidean space with its standard symplectic structure ω_0. We call a symplectic form translationally invariant if its matrix has the same form at any point on the manifold.

Now we turn to symplectic transformations between symplectic manifolds. We will use hereafter interchangeably the notions of symplectic transformations, symplectic maps, canonical transformations, symplectic diffeomorphisms and symplectomorphisms. By definition, a diffeomorphism $\mathcal{M} : P_1 \to P_2$ between two symplectic manifolds (P_1, ω_1) and (P_2, ω_2) of the same dimension is called a symplectomorphism if it preserves the symplectic forms, that is

$$\mathcal{M}^* \omega_2 = \omega_1, \tag{2}$$

where * denotes the pull-back, which is defined as

$$(\mathcal{M}^* \omega)_z (v_1, v_2) = \omega_{\mathcal{M}(z)} (T_z \mathcal{M} \cdot v_1, T_z \mathcal{M} \cdot v_2), \tag{3}$$

where $z \in P_1$ and $v_1, v_2 \in T_m P_1$. In this case P_1 and P_2 are said to be symplectomorphic. In canonical coordinates this definition takes the following form for a symplectic map of the Euclidean space with its standard symplectic structure ω_0

$$(\mathrm{Jac}(\mathcal{M}))^T J (\mathrm{Jac}(\mathcal{M})) = J. \tag{4}$$

Here Jac denotes the Jacobian and ^{T} the matrix transpose. The above definition can be extended to include conformal symplectic maps by the following relation

$$\mathcal{M}^* \omega_2 = r(\mathcal{M}) \omega_1, \tag{5}$$

with $r(\mathcal{M}) \in \mathbb{R}^\times$. To see the significance of r, take a scaling map defined by $\phi^* \omega_1 = \mu^2 \omega_1$, $\mu \in \mathbb{R}^\times$ and apply it to both sides of (5). By choosing $\mu = 1/\sqrt{|r|}$, we obtain $(\mathcal{M} \circ \phi)^* \omega_2 = \mathrm{sgn}(r(\mathcal{M})) \omega_1$. Hence, if $r > 0$, then $\mathcal{M} \circ \phi$ is symplectic. If $r < 0$, then $\mathcal{M} \circ \phi$ is called antisymplectic. Essentially, it means that $\mathcal{M} \circ \phi$ is orientation reversing. Actually, this is strictly true only if n is odd, otherwise, for n even, the Cartesian product $(\mathcal{M} \circ \phi) \times \mathcal{I}$ is orientation reversing; $\mathcal{I}$ being the identity map. This follows from the definition of the symplectic map. Specifically, any symplectic map of a manifold into itself preserves the symplectic form, so it also preserves the volume form $\omega^n = \omega \wedge ... \wedge \omega$ (n times). This is a never vanishing $2n$-form on a $2n$ dimensional manifold, so the vector space it forms is 1 dimensional. Direct calculation shows that it integrates to a constant times the Euclidean volume. It follows that any symplectic manifold is oriented by the volume form, symplectic maps preserve orientation, and if global coordinates are available the determinant of the Jacobian of any symplectic map is equal to 1 at any point.

Now we turn our attention to Hamiltonian systems, as the dynamics of interest to us can be described to a very good level of approximation by a Hamiltonian dynamical system. First we establish a few notations. Obviously, the symplectic maps of a symplectic manifold form an infinite dimensional Lie group under composition, denoted by $\mathrm{Symp}(P, \omega) \equiv \mathrm{Symp}(P)$, if it is clear which symplectic form is considered. Also its Lie algebra of symplectic vector fields will be denoted by $\mathcal{X}(P)$. In the view of non-degeneracy of symplectic forms, there is a one-to-one correspondence between vector fields and 1-forms via

$$\mathcal{X}(P) \to \Omega^1(P) : X \to \imath(X) \omega, \tag{6}$$

where we used $\imath$ for the interior product. A vector field X is called symplectic if $\imath(X) \omega$ is closed, that is $d(\imath(X) \omega) = 0$. By the Poincaré lemma, on connected manifolds every closed 1-form is locally exact, so $\imath(X)\omega$ can be written locally as the differential of a function $\imath(X)\omega = dH$. In this case the vector field is called locally Hamiltonian. If dH exists globally (for example if the manifold is simply connected), X is called Hamiltonian, and H the Hamiltonian function. Conversely, for any function $H : P \to \mathbb{R}$, the vector field $X_H : P \to TP$ determined by the identity $\imath(X_H)\omega = dH$ is called the Hamiltonian vector field associated to the Hamiltonian function H. A Hamiltonian dynamical system is the triple (P, ω, H). Hamiltonian vector fields form a Lie subalgebra of the Lie algebra of symplectic vector fields. The map $X_H \to H$ is a homomorphism. However, if we restrict ourselves to compactly supported Hamiltonians, then the map becomes an isomorphism, and it can be viewed as a normalization condition, by specifying the arbitrary constant in H. With this normalization different Hamiltonians generate different flows. Specifically, compact support means that the Hamiltonian and hence the associated vector field vanishes outside a compact subset. Recall that vanishing Hamiltonians generate the identity map. Hence, the support of a symplectic map is defined as the closure of the set where it is different from identity.

To define Hamiltonian symplectomorphisms we need first the notion of isotopy. The time-dependent vector field X_{H_t}, associated to the time-dependent Hamiltonian H_t at every t, generates a smooth 1-parameter group of diffeomorphisms $\phi^t_{H_t}$ satisfying

$$\frac{d}{dt}\phi^t_{H_t} = X_{H_t} \circ \phi^t_{H_t} \quad , \quad \phi^0_{H_t} = \mathcal{I}. \tag{7}$$

$\phi^t_{H_t}$ is called the Hamiltonian flow associated to H_t, or the Hamiltonian isotopy. A symplectomorphism $\phi \in \mathrm{Symp}(P)$ is called Hamiltonian if there exists a Hamiltonian isotopy $\phi_t \in \mathrm{Symp}(P)$ from $\phi_0 = \mathcal{I}$ to $\phi_1 = \phi$. We denote the space of Hamiltonian symplectic maps by $\mathrm{Ham}(P, \omega)$, or simply $\mathrm{Ham}(P)$. It turns out that $\mathrm{Ham}(P)$ is a normal subgroup of $\mathrm{Symp}(P)$, and its Lie algebra is the Lie algebra of Hamiltonian vector fields. On simply connected manifolds $\mathrm{Ham}(P)$ is the identity component of $\mathrm{Symp}(P)$, that is any symplectic isotopy is Hamiltonian [12]. The group of Hamiltonian symplectomorphisms is path connected. Also, any path in the space of Hamiltonian maps is Hamiltonian. If a symplectic map is generated by compactly supported Hamiltonians, the symplectic map is also compactly supported, which means that it is the identity map outside a compact subset.

To prove that the flows of Hamiltonian systems are symplectic we need the following two formulae [13]: the Lie derivative formula

$$\frac{d}{dt}\phi_t^*\omega = \phi_t^*\mathcal{L}_{X_t}\omega, \tag{8}$$

and Cartan's magic formula

$$\mathcal{L}_{X_t}\omega = \imath(X_t)\,d\omega + d\left(\imath(X_t)\,\omega\right). \tag{9}$$

Now it is straightforward to see that if $d\omega = 0$ and $(\imath(X_t)\omega) = dH_t$, then $\frac{d}{dt}\phi_t^*\omega = 0$, that is constant in time and equal to its value at $t = 0$. Hence we obtain $\phi_t^* \omega = \omega$, for any t. The argument works also backwards, implying that if the flow of a dynamical system is symplectic then it is generated by Hamiltonian dynamical systems.

2.2 Primitive Function vs. Generating Function

In this subsection it is shown that the main ideas of mixed variable generating functions are already built in in the symplectic condition. Consider symplectic transformations, $\mathcal{M}$, of a symplectic manifold (T^*X, ω). Let us assume that the manifold is simply connected, or in other words is an exact symplectic manifold. Then, every closed form is also exact. We can write $\omega = -d\lambda$. The symplectic condition takes the form

$$d\left(\lambda - \mathcal{M}^* \lambda\right) = 0, \tag{10}$$

from which follows the existence of a function F, such that

$$\lambda - \mathcal{M}^* \lambda = dF. \tag{11}$$

The function F is called the primitive function of $\mathcal{M}$. However, there is no one-to-one correspondence between symplectic maps and primitive functions. Actually, the symplectic map is determined up to a left action (composition with $\mathcal{M}$ from the left) of an actionmorphism, i.e. a symplectic map that preserves the 1-form λ. This can be easily seen by replacing $\mathcal{M}$ with another symplectic map, $\mathcal{N} \circ \mathcal{M}$, where $\mathcal{N}$ an actionmorphism. Therefore, we obtain

$$\begin{aligned} \lambda - \left(\mathcal{N} \circ \mathcal{M}\right)^* \lambda &= \lambda - \mathcal{M}^* \left(\mathcal{N}^* \lambda\right) &(12)\\ &= \lambda - \mathcal{M}^* \lambda &(13)\\ &= dF. &(14) \end{aligned}$$

Hence, $\mathcal{M}$ and $\mathcal{N} \circ \mathcal{M}$ have the same primitive function. All the $\mathcal{N}$s with this property arise as lifts of diffeomorphisms on the base manifold [13]. Therefore, the primitive function determines the symplectic maps up to cotangent lifts. This is a manifestation of the coordinate independence of the symplectic condition, specifically λ. It also implies that for one-to-one correspondence between $\mathcal{M}$ and F, F cannot be defined on phase space.

If we think of $(\vec{q}, \vec{p})$ as independent canonical coordinates, and $\mathcal{M}(\vec{q}, \vec{p}) = \left(\vec{Q}, \vec{P}\right)$, it follows from (11) that

$$\vec{p} \cdot d\vec{q} - \vec{P} \cdot d\vec{Q} = dF\left(\vec{q}, \vec{p}\right). \tag{15}$$

Now, if the equation $\vec{Q} = \vec{Q}\left(\vec{q}, \vec{p}\right)$ can be solved for $\vec{p}$ to give a function $F_1\left(\vec{q}, \vec{Q}\right) = F\left(\vec{q}, \vec{p}\left(\vec{q}, \vec{Q}\right)\right)$, with $\left(\vec{q}, \vec{Q}\right)$ as independent variables, we obtain

$$\frac{\partial F_1\left(\vec{q}, \vec{Q}\right)}{\partial \vec{q}} = \vec{p} \quad , \quad \frac{\partial F_1\left(\vec{q}, \vec{Q}\right)}{\partial \vec{Q}} = -\vec{P}, \tag{16}$$

and we recognize it as the F_1 (Goldstein type 1) generating function. The symplectic maps with this property are called twist maps.

Now it is apparent that, in order to uniquely determine the symplectic map, a function must employ mixed variables, and this follows from the symplectic condition itself. The method used in this section could be used to derive other types of generating functions. However, there are many λs such that $\omega = -d\lambda$, as for example $\lambda = -\vec{q} \cdot d\vec{p}$ or $\lambda = \frac{1}{2}(\vec{p} \cdot d\vec{q} - \vec{q} \cdot d\vec{p})$, etc. Moreover, different λs can be chosen on the source and target manifold, and guessing is necessary for the variable changes. Therefore, it is not clear how much freedom is possible for construction of new generating functions, and in general it is not convenient to work in this setting. We choose to work in another setting, which has been introduced by Weinstein.

2.3 Symplectic Maps as Lagrangian Submanifolds

Initially, we have symplectic maps of a manifold in one hand, and functions on another manifold on the other hand. The local representative of the symplectic maps are vector functions of an even number of components. Our generating function is a scalar function. A priori, the most general method to connect the two in a one-to-one manner is not clear. In the early '80s Weinstein formulated a "symplectic creed" with the motto "in symplectic geometry everything is a Lagrangian submanifold" (see definition below). Indeed, in symplectic geometry Lagrangian submanifolds are the most important objects beside the symplectic manifolds themselves. These Lagrangian submanifolds provide the most general link between symplectic maps and generating functions. Both symplectic maps, and functions under certain conditions, can be put in one-to-one correspondence with Lagrangian submanifolds of appropriate symplectic manifolds. Once this correspondence is established, instead of working at the level of symplectic maps and functions we can work with Lagrangian submanifolds. At this point, the link we are looking for will be given by the most general type of diffeomorphisms that map these Lagrangian submanifolds into each other, or in other words the diffeomorphisms of identification of the two Lagrangian submanifolds.

We will consider only submanifolds of symplectic manifolds that are properly embedded and which inherit their topology from the ambient manifold. Also, we will need to work with injections of graphs of maps. It can be proved that the graph of a smooth map $f : P_1 \to P_2$,

$$\Gamma_f = \{(f(p), p) \ | \ p \in P_1, \ f(p) \in P_2\} \subset P_1 \times P_2 \tag{17}$$

is a smooth submanifold of $P_1 \times P_2$ of dimension $\dim(P_1)$ [13]. Moreover, if f is a diffeomorphism, then the projections $\pi_i : \Gamma_f \to P_i$, $i = 1, 2$ are diffeomorphisms [13, 14].

Lagrangian submanifolds are defined in terms of tangent spaces on which the symplectic form vanishes.

Definition 1 *Let (P, ω) be a $2n$ dimensional symplectic manifold and let L be a submanifold of P. L is called a Lagrangian submanifold if, at each $p \in L$, T_pL*

is a Lagrangian subspace of T_pP*, i.e.* $\omega_p|_{T_pL} \equiv 0$ *and* $\dim T_pL = \frac{1}{2}\dim T_pP$*. Equivalently, if* $i : L \hookrightarrow P$ *is the inclusion map, then* L *is Lagrangian if and only if* $i^*\omega = 0$ *and* $\dim L = \frac{1}{2}\dim P$*.*

First we prove that any symplectic map $\mathcal{M} : (P_1, \omega_1) \to (P_2, \omega_2)$, $\mathcal{M}^*\omega_2 = \omega_1$, can be interpreted as a Lagrangian submanifold in the Cartesian product space $P_2 \times P_1$ with the symplectic structure $\mu(\pi_2^*\omega_1 - \pi_1^*\omega_2)$, where $\pi_i : P_2 \times P_1 \to P_i$, $i = 1, 2$, are the canonical projections and $\mu \in \mathbb{R}^\times$. The graph of the symplectic map is the $2n$-dimensional submanifold of $P_2 \times P_1$

$$\Gamma_{\mathcal{M}} = \{(\mathcal{M}(z), z) \mid z \in P_1\}. \tag{18}$$

Denote $P = P_2 \times P_1$ and $\omega = \mu(\pi_2^*\omega_1 - \pi_1^*\omega_2)$; then we have the following:

Theorem 2 $\mathcal{M}$ *is a symplectomorphism if and only if* $\Gamma_{\mathcal{M}}$ *is a Lagrangian submanifold of* (P, ω)*.*

Proof. $\Gamma_{\mathcal{M}}$ is Lagrangian iff relative to the inclusion map $i : \Gamma_{\mathcal{M}} \hookrightarrow P$, $i^*\omega = 0$.

$$\begin{aligned} i^*\omega &= \mu(i^*\pi_2^*\omega_1 - i^*\pi_1^*\omega_2) & (19)\\ &= \mu\left((\pi_2 \circ i)^*\omega_1 - (\pi_1 \circ i)^*\omega_2\right) & (20)\\ &= \mu(\mathcal{I}^*\omega_1 - \mathcal{M}^*\omega_2) & (21)\\ &= \mu(\omega_1 - \mathcal{M}^*\omega_2) = 0. & (22) \end{aligned}$$

Hence, because $\mu \neq 0$, it follows that $\mathcal{M}^*\omega_2 = \omega_1$. ■

Arbitrary Lagrangian submanifolds of (P, ω) are called canonical relations, and can be considered as generalizations of symplectic maps. For practical applications we will be interested in the case $P_1 = P_2 = \mathbb{R}^{2n}$, and $\omega_1 = \omega_2 = \omega_0$ being the standard symplectic structure of $\mathbb{R}^{2n}$. Thus, in this case, any symplectic map $\mathcal{M} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is a Lagrangian submanifold in $\left(\mathbb{R}^{4n}, \mu\tilde{\mathbb{J}}\right)$, with symplectic structure ω that has the matrix

$$\mu\tilde{J} = \mu\begin{pmatrix} J_{2n} & 0_{2n} \\ 0_{2n} & -J_{2n} \end{pmatrix}. \tag{23}$$

One particular Lagrangian submanifold of this kind that will be useful later is the diagonal, which by definition is the graph of the identity map

$$\Delta = \{(z, z) \mid z \in P_1\}. \tag{24}$$

2.4 Functions as Lagrangian Submanifolds

Next, we turn our attention to the one-to-one correspondence that can be set up between closed one-forms and Lagrangian submanifolds of cotangent bundles that project diffeomorphically onto the base manifold. Consider a smooth manifold X and a 1-form defined on it. Regard it as a map from X to T^*X. Then the following holds:

Proposition 3 *The canonical one-form* $\lambda \in \Omega^1 (T^*X)$ *is uniquely characterized by the property that*

$$\sigma^* \lambda = \sigma, \tag{25}$$

for every one-form $\sigma : X \to T^*X$.

Proof. The σ on the left hand side is considered as a map, and on the right hand side as a one-form. Denote the coordinates of T^*X by $(\vec{q}, \vec{p})$. Then σ regarded as a map in these coordinates can be written as $\sigma = \left(\vec{q}, \vec{f}(\vec{q})\right)$ for some functions f_i. Recall that the canonical one-form has the expression $\lambda = \vec{p} \cdot d\vec{q}$. Thus, using the definition of the pull-back we obtain

$$\begin{aligned} (\sigma^* \lambda)_{\vec{q}} &= \lambda_{\sigma(\vec{q})} \cdot d_{\vec{q}} \sigma & (26) \\ &= \begin{pmatrix} \sigma_{\vec{q}} \\ 0 \end{pmatrix}^T \begin{pmatrix} I \\ d_{\vec{q}} \vec{f}(\vec{q}) \end{pmatrix} & (27) \\ &= \sigma_{\vec{q}}. & (28) \end{aligned}$$

where we used that $\lambda_{\sigma(\vec{q})} = \left(\vec{p} \circ \vec{f}(\vec{q})\right) \cdot d(\vec{q} \circ \vec{q}) = \vec{f}(\vec{q}) \cdot d\vec{q} = \sigma_{\vec{q}}$, $(\vec{q}, \vec{p})$ being regarded as components of the identity map. ■

Now we demonstrate that when σ is closed, its image $\sigma(X)$ (σ regarded as a map) is a Lagrangian submanifold of T^*X with the standard symplectic structure. Note that the graph Γ_σ of the one-form σ is defined as

$$\Gamma_\sigma = \{(\sigma(w), w) \mid w \in X, \sigma(w) \in T_w^* X\}. \tag{29}$$

Its image by the inclusion $i : \Gamma_\sigma \to T^*X$ is Lagrangian. Relative to the projection $\pi : \Gamma_\sigma \to X$, Γ_σ is uniquely determined by the one-form σ if and only if π is a diffeomorphism. This can be seen from the fact that $i = \sigma \circ \pi$. Hence, Γ_σ is Lagrangian iff $i^* \omega_0 = 0$. Thus we get

$$\begin{aligned} (\sigma \circ \pi)^* \omega_0 = (\sigma \circ \pi)^* (-d\lambda) &= -\pi^* (d(\sigma^* \lambda)) & (30) \\ &= -\pi^* d\sigma = 0, & (31) \end{aligned}$$

where we used $\omega_0 = -d\lambda$, the fact that the pull-back commutes with the exterior differential and the result of the above proposition. Therefore, there is a one-to-one correspondence between Lagrangian submanifolds of $(T^*X, \nu\omega_0)$ of the form (29) which project diffeomorphically onto X, and closed one-forms σ on X; here $\nu \in \mathbb{R}^\times$.

In general, there are two ways to ensure that π is a diffeomorphism; if the embedding is C_1 close enough (i.e. close enough in norm to the function values as well as the values of the first derivatives) to the canonical embedding of the zero section into the cotangent bundle, or σ (as the differential of a function) is a diffeomorphism. In the first case the projection mapping will be C_1 close enough to identity to be a diffeomorphism. Indeed, it can be showed [10] that if

$$\| df - \mathcal{I} \| \leq \frac{1}{2}, \tag{32}$$

then f is a diffeomorphism. Hence, in this case π can be guaranteed to be a diffeomorphism if σ is C_1 close enough to 0.

For example, the zero section of T^*X, defined by

$$Z = \{(\xi, w) \mid \xi = 0, w \in X, \xi \in T^*_w X\} = \{0\} \times X \tag{33}$$

is such a Lagrangian submanifold. This obviously follows from the fact that $\xi = 0$, so $\lambda|_Z = 0$.

Other examples of Lagrangian submanifolds are the fibers of cotangent bundles ("delta functions" at a fixed point in the base manifold), any smooth curve on a 2 dimensional symplectic manifold, invariant tori (KAM tori) of Hamiltonian systems, etc.

The next step is to make the connection between functions on X and the Lagrangian submanifolds of the form (29) of T^*X. This is possible if the one-form σ is exact, that is can be written as the differential of a function. The condition when this is possible can be described by the first Betti number. First we define the de Rham cohomology groups $H^k(X, \mathbb{R})$ by

$$H^k(X, \mathbb{R}) = \frac{\ker\left(d : \Omega^k(X) \to \Omega^{k+1}(X)\right)}{\operatorname{range}\left(d : \Omega^{k-1}(X) \to \Omega^k(X)\right)}. \tag{34}$$

The elements of $H^k(X, \mathbb{R})$ form a vector space, and its dimension is called the k-th Betti number

$$b_k = \dim H^k(X, \mathbb{R}), \tag{35}$$

which measures the failure of closed forms to be globally exact. On the other hand, if X is connected, by the Poincaré lemma every closed form is locally exact. If $b_1 = 0$, it follows that every closed one-form is globally the differential of a function. In this case the closed one-form σ can be written as dF for a function F that is unique up an additive arbitrary constant. The function $F \in \mathcal{F}(C^\infty(X))$ is called the generating function of the Lagrangian submanifold Γ_σ. Hence, if $b_1 = 0$ we can think of Lagrangian submanifolds Γ_σ as generalized functions on X. We note the well-known fact that for $\mathbb{R}^{2n}$, $b_0 = 1$ and $b_i = 0$ for $i \geq 1$. In the case relevant for our applications, in Euclidean space, every function "generates" a Lagrangian submanifold, and conversely, given a Lagrangian submanifold of the form (29), which projects diffeomorphically onto the base manifold, its generating function can be computed by mere integration along an arbitrary path. Also, this function will be called the generating function of the canonical transformation. However, it is still necessary to link the Lagrangian submanifolds (18) and (29) with suitable diffeomorphisms. We do that in the next subsection.

We mention that the projection π is actually a fiber translation, and Γ_σ intersects each fiber at most in only one point. The fact that Γ_σ might not project diffeomorphically is a hint that some generating functions do not exist for certain symplectic maps. In the case that the projection is not a global diffeomorphism, we certainly cannot have a global generating function, but still it might be possible to define a local generating function, if the origin has a neighborhood that projects diffeomorphically. While, for special cases of symplectic maps and types of generating functions it might be possible to ensure that the projection is a global diffeomorphism (see for example twist maps and Goldstein type 1 generating functions), in general the projection can be guaranteed to be a global diffeomorphism only if Γ_σ is close enough to the zero section. In this case, the projection map is C^1-close enough to identity to be a diffeomorphism. Hence, every C^2-small enough function is in one-to-one correspondence with such a Lagrangian submanifold. At this point it is not clear how much freedom we have to map Lagrangian submanifolds into each other, but it is a basic requirement of the theory to try to map as close to the zero section as possible.

2.5 Existence of Infinitely Many Generating Functions

Now we are ready to link symplectic maps with their generating functions. The most natural and general way is to require the Lagrangian submanifold determined by a function to be diffeomorphic to the Lagrangian submanifold determined by the symplectic map, if such a map exists. A well-known theorem [15] states that a neighborhood of any Lagrangian submanifold can be identified by a local symplectomorphism with a neighborhood of the zero section in the cotangent bundle of the submanifold. In general there are two difficulties with this approach. If the manifolds are not simply connected, the generating functions in general cannot be defined globally, and from the computational point of view, it is difficult to deal with the complicated cotangent bundles of the Lagrangian submanifolds determined by the symplectic maps. That is why in general this approach is best suited for symplectic maps close to identity. Also, the theorem states the existence of a local symplectomorphism that identifies the appropriate Lagrangian submanifolds, but is not a priori clear that this is the most general way to do that. Fortunately, for our purpose it is enough to consider only the case of Euclidean space, for which more results can be obtained.

If we are limiting ourselves to simply connected manifolds, and if it happens that P_i, $i = 1, 2$, are diffeomorphic to X, then we have the following commutative diagram:

$$\begin{array}{ccc} \Gamma_{\mathcal{M}} & \xrightarrow{\alpha} & \Gamma_{dF} \\ \pi_i\downarrow & & \downarrow\pi \\ P_i & \xrightarrow{\varphi_i} & X \end{array} \tag{36}$$

$\mathcal{M}$ being a symplectomorphism, the projections π_i are diffeomorphisms. Moreover, it is assumed that π is a diffeomorphism, and there exist a diffeomorphism $\varphi_i : P_i \to X$. Thus, in this case there exists a diffeomorphism $\alpha : \Gamma_{\mathcal{M}} \to \Gamma_{dF}$, for any pair of Lagrangian submanifolds of this form, satisfying the above conditions. The following theorem [16, 17] shows that α extends to a local symplectomorphism. It can be thought of as a generalization of the main theorem of [15].

Theorem 4 *Let L_i be two Lagrangian submanifolds of the symplectic manifolds (P_i, ω_i), $i = 1, 2$. Then **any** diffeomorphism $\alpha : L_1 \to L_2$ extends to a conformal* *symplectomorphism $\beta : U_1 \to U_2$ of some neighborhoods U_i of L_i in P_i, such that $\beta|_{L_1} \equiv \alpha$.*

Consider the following diagram:

$$
\begin{tikzcd}
 & (P,\omega) \arrow[rrr, "\beta"] & & & (T^*X,\nu\omega_0) & \\
 & \Gamma_{\mathcal{M}} \arrow[u, "i_{\mathcal{M}}"] \arrow[dl, "\pi_2 \circ i_{\mathcal{M}}"'] \arrow[dr, "\pi_1 \circ i_{\mathcal{M}}"] \arrow[rrr, "\alpha"] & & & \Gamma_{dF} \arrow[u, "i_{dF}"'] \arrow[dl, "\pi"'] & \\
 z \arrow[rr, "\mathcal{M}"] & & \mathcal{M}(z) & w \arrow[rr, "dF"] & & dF(w) \arrow[ul, "i"']
\end{tikzcd}
$$

where $z \in P_1$ and $w \in X$ are arbitrary points of the respective manifolds.

We pointed out that the local classification, around a point, of symplectic structures is completely solved by Darboux's theorem. Here we have another concept of locality, namely local around a submanifold, of which one can think of as germs of the symplectic manifolds. Marle's theorem is an example of such a tubular theorem, first proved to exist by Weinstein. It says that Lagrangian submanifolds do not have geometric invariants in order to distinguish each other. In general there are no global theorems similar to the tubular ones. This is true even in the $\mathbb{R}^{2n}$ case, due to the existence of exotic symplectic structures proved by Gromov [18].

The importance of the above theorem consists of two main aspects: it gives the most general way to represent symplectic maps globally by scalar functions, and implies that once a symplectomorphism β exists for a symplectic map $\mathcal{M}$ and a function F, it is automatically valid for all nearby symplectic maps. It follows that the freedom for selecting generating function types is given by the set of conformal symplectic maps of the form $\beta^*\omega_0 = \omega/\nu$. A generating function of type α, which exists for a given $\mathcal{M}$, exists for all nearby symplectic maps. In case the assumptions of the theorem are satisfied, any Lagrangian submanifold $\Gamma_{\mathcal{M}}$ can be identified with any Lagrangian submanifold Γ_{dF}; therefore, in principle the scalar function F can always be chosen in such a way that π is a diffeomorphism, guaranteeing global generating function types for any symplectic map. Clearly, once α is fixed, there is a one-to-one correspondence between symplectic maps and functions, hence they are called the generating functions of the symplectic maps. Interestingly enough, the diagram shows that, when the theorem's conditions hold, to any pair $(\mathcal{M}, F)$ can be found an α (which is not unique) such that F becomes the generating function of type α of $\mathcal{M}$. Also, generating functions can be defined on any simply connected manifold X diffeomorphic to P_i, and as mentioned above, β cannot in general be extended to a global conformal symplectic map.

Now we specialize these result to the case of Euclidean spaces. Notice that for our practical cases in dynamics $\mathcal{M} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, and it is computationally convenient to define the generating functions also on $\mathbb{R}^{2n}$. Hence $P_1 = P_2 = X = \mathbb{R}^{2n}$, and $\omega_1 = \omega_2 = \omega_0$. As long as π is a diffeomorphism, the theorem applies and the existence of the diffeomorphism α, which can be extended to a local symplectomorphism β follows. Global canonical coordinates are available, in which the symplectic structures ω and $\nu\omega_0$ are translationally invariant with matrices, $\mu\tilde{J}$ and νJ respectively. Therefore, there is an α which can be used to identify any Lagrangian submanifold of $\left(\mathbb{R}^{4n}, \mu\tilde{\mathbb{J}}\right)$ of the form (18) with any Lagrangian submanifold of $\left(\mathbb{R}^{4n}, \nu\mathbb{J}\right)$ of the form (29). According to the theorem, the most general form of β is a conformal symplectic map. Since α is the restriction of β to the Lagrangian submanifolds, we conclude that the most general form of the diffeomorphism α that links the symplectic maps to their generating functions is

$$\alpha^* \omega_0 = \frac{1}{\nu}\omega. \tag{37}$$

In fact, this was expected from the local theory. The global theory just states that instead of matrices nonlinear maps can be used, and the local maps around each point can be glued together along germs of Lagrangian submanifolds, which entail the existence of global generating function types.

In conclusion, we have the following fundamental results in the case of Euclidean space: there is a one-to-one correspondence between any small function (in the C^2 sense) $F \in \mathcal{F}\left(C^\infty\left(\mathbb{R}^{2n}\right)\right)$ and symplectic map $\mathcal{M} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, realized through a diffeomorphism $\alpha : \Gamma_{\mathcal{M}} \to \Gamma_{dF}$ such that

$$\Gamma_{dF} = \alpha\left(\Gamma_{\mathcal{M}}\right), \tag{38}$$

$$\alpha^* \omega_0 = \frac{1}{\nu}\omega. \tag{39}$$

For a fixed α, the function F that satisfies the above equations is called the generating function of type α of the canonical transformation represented by $\mathcal{M}$. The same type of generator exists for all symplectic maps close enough to each other (in the C^1 topology). Obviously, from these equations it follows that to every symplectic map infinitely many generating functions can be constructed, due to the fact that the Lie group of diffeomorphisms of the form (39) contains infinitely many elements.

This completes the global theory of generating functions. It is worthwhile to note that the theory is global in the sense that guarantees the existence of global generating functions for any symplectic map. However, it is local in the sense that it proves that one fixed type of generator cannot exist for all symplectic maps, not even locally around a point.

3 Generating Functions from the Computational Point of View

This section presents a computationally convenient method to obtain generating functions of given symplectic maps. First, it is necessary to rewrite (38-39) in a form that is convenient computationally. The vector function associated to the one-form dF by the standard Euclidean scalar product is the gradient, ∇F.

We write $\mathcal{N} = (\nabla F)^T$ for the map, regarded as a column vector, represented by ∇F. "$d\mathcal{N} = 0$" means that

$$\frac{\partial \mathcal{N}_i}{\partial w_j} = \frac{\partial \mathcal{N}_j}{\partial w_i}, \quad i, j = 1, ..., 2n. \tag{40}$$

These are the well-known necessary and sufficient conditions for the existence of a scalar potential [6]. The generating function is the potential of the closed one-form that determines the Lagrangian submanifold.

Denote some canonical coordinates by $z = (\vec{q}, \vec{p})$, and denote the coordinates of the space where the generating function is defined by w. Introduce $\hat{z}$ and $\hat{w}$ by $\hat{z} = \mathcal{M}(z)$ and $\hat{w} = \mathcal{N}(w)$. Then (38) can be expressed as

$$\begin{pmatrix} \hat{w} \\ w \end{pmatrix} = \alpha \begin{pmatrix} \hat{z} \\ z \end{pmatrix}, \tag{41}$$

$$\begin{pmatrix} \mathcal{N}(w) \\ w \end{pmatrix} = \alpha \begin{pmatrix} \mathcal{M}(z) \\ z \end{pmatrix}. \tag{42}$$

Splitting α into the first $2n$ and last $2n$ components, we obtain

$$\alpha = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}. \tag{43}$$

Similarly, for its inverse α^{-1} we write

$$\alpha^{-1} = \begin{pmatrix} \alpha^1 \\ \alpha^2 \end{pmatrix}. \tag{44}$$

From (42) it follows that

$$w = \alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix} (z), \tag{45}$$

$$\mathcal{N}(w) = \alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix} (z). \tag{46}$$

Combining the two equations we obtain that

$$\mathcal{N} \circ \alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix} (z) = \alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix} (z). \tag{47}$$

Requiring $\alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}$ to be invertible, in terms of maps we obtain the following formula, useful for the actual computation of the generating function:

$$(\nabla F)^T = \left(\alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}\right) \circ \left(\alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}\right)^{-1}. \tag{48}$$

Therefore, the similar formula that has been defined in the local theory, without apparent deep logic behind it, is recovered, and the general condition that requires π to be a diffeomorphism appears in computations as the above mentioned invertibility condition. If the respective map does not have a global inverse, clearly there is no global generating function. Obviously, the symplectic map $\mathcal{M}$ needs to be defined globally. If (45) fails to be a global diffeomorphism, there is still a chance to be defined locally, producing local generators. The invertibility condition sometimes is called the transversality condition. Locally, around the origin, this is satisfied whenever

$$\det\left(\operatorname{Jac}\left(\alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}(z)\big|_{z=0}\right)\right) \neq 0. \tag{49}$$

Denote the Jacobian of α by $\alpha_{\#} = \operatorname{Jac}(\alpha)$. $\alpha_{\#}$ can be written as

$$\alpha_{\#} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{50}$$

A, B, C, D being $2n \times 2n$ block matrices. Hence, assuming that the symplectic maps are origin preserving, i.e. $\mathcal{M}(0) = 0$, the local transversality condition around the origin is

$$\det\left(C(0,0) \cdot M(0) + D(0,0)\right) \neq 0, \tag{51}$$

where $M = \operatorname{Jac}(\mathcal{M})$. If this necessary condition is satisfied, then the generating function is defined in a neighborhood of the origin, and can be calculated from (48) by mere integration along an arbitrary path. The arbitrariness of the path is assured by Stokes' theorem.

We note that in fact the computation of F according to (48), and subsequent integration, gives F, which is the primitive function rather than the generating function. To get the generating function itself, one has to keep in mind to which α it is associated, and compute F in the w coordinates,

$$F \longmapsto F \circ \left(\alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}\right). \tag{52}$$

There is a nice geometric interpretation of the global existence of the generating functions. As has been seen, any Lagrangian submanifold in unique correspondence with $\mathcal{M}$ can be sent diffeomorphically onto the Lagrangian submanifold determined by F. If, for some choice of α, this is achieved in such a way that Γ_{dF} is close enough to the zero section to project diffeomorphically onto the base, the generating function of type α exists globally. Recall that the group of diffeomorphisms is open in the set of smooth maps in the C^1 topology. Therefore, any smooth map close enough to the identity is a global diffeomorphism [12]. The reflection of this fact is that $\alpha_2(\hat{z}, z)$ has a global inverse. However, it might not be possible in practice to find an α satisfying this condition, especially for very nonlinear symplectic maps, and we need to consider local generating functions. If the projection diffeomorphisms are local, defined in a neighborhood of the origin, then we have local generating functions. In this case, one can think intuitively that fixing the type of generating function, as the nonlinearities of the symplectic map increase, the singularities move closer to the origin, limiting the domain of validity of the generating function. However, we always assume that the dynamics is taking place in a finite region of the phase space, so there is no loss of generality in assuming that the symplectic maps are compactly supported, and requiring only that the generating function to be defined in the region of interest. If the symplectic maps are too "big" for the generating functions to cover the region of interest, the problem can always be alleviated by taking roots of the symplectic map.

Next, we are interested in the constraints imposed by α. Equation (39) written in coordinates is

$$\alpha_{\#}^T J_{4n} \alpha_{\#} = \frac{\mu}{\nu} \tilde{J}_{4n}. \tag{53}$$

By abuse of notation, for μ/ν we write $\mu \in \mathbb{R}^\times$. More explicitly (53) reads

$$\begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \begin{pmatrix} 0_{2n} & I_{2n} \\ -I_{2n} & 0_{2n} \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \mu \begin{pmatrix} J_{2n} & 0_{2n} \\ 0_{2n} & -J_{2n} \end{pmatrix}, \tag{54}$$

which gives the constraints

$$A^T C - C^T A = \mu J_{2n}, \tag{55}$$
$$B^T D - D^T B = -\mu J_{2n}, \tag{56}$$
$$A^T D - C^T B = 0. \tag{57}$$

Knowing that α is a diffeomorphisms, obviously $\alpha_{\#}$ is invertible. It is easy to see that $\det(J_{4n}) = 1$ and $\det\left(\tilde{J}_{4n}\right) = \det(J_{2n}) \cdot \det(-J_{2n}) = 1$, and hence $(\det(\alpha_{\#}))^2 = \mu^{4n} \neq 0$. Then equivalently, (53) can be written as follows:

$$\alpha_{\#}^T J_{4n} = \mu \tilde{J}_{4n} \alpha_{\#}^{-1}. \tag{58}$$

Transposition gives

$$J_{4n} \alpha_{\#} = \mu \alpha_{\#}^{-T} \tilde{J}_{4n}, \tag{59}$$

where we used $J_{4n}^T = -J_{4n}$ and $\tilde{J}_{4n}^T = -\tilde{J}_{4n}$. Obviously, $J_{4n}^{-1} = -J_{4n}$ and $\tilde{J}_{4n}^{-1} = -\tilde{J}_{4n}$, so it results that

$$J_{4n} \alpha_{\#} \tilde{J}_{4n} = -\mu \alpha_{\#}^{-T}, \tag{60}$$
$$J_{4n} \alpha_{\#} \tilde{J}_{4n} \alpha_{\#}^T = -\mu, \tag{61}$$
$$\alpha_{\#} \tilde{J}_{4n} \alpha_{\#}^T = \mu J_{4n}, \tag{62}$$

which gives the equivalent set of constraints, but better suited for further analysis:

$$A J_{2n} A^T - B J_{2n} B^T = 0, \tag{63}$$
$$C J_{2n} C^T - D J_{2n} D^T = 0, \tag{64}$$
$$D J_{2n} B^T - C J_{2n} A^T = \mu I_{2n}. \tag{65}$$

The constraints show that (A, B) and (C, D) must be symplectic pencils, and there is an additional condition that links the two pencils.

An important observation is that in the process of construction of the generating function from a symplectic map (63-65) have to be satisfied exactly. This means that we need to construct αs that are exact conformal symplectic maps. On computers it is most convenient to work with polynomial maps. To our knowledge, the classification of polynomial symplectic maps is not known. If we constrain ourselves to consider linear maps α, they can be easily constructed and represented exactly on a computer. In this case α can be represented by a $4n \times 4n$ constant matrix. If A is invertible, it follows that $A^{-1}B$ is a symplectic matrix. The same argument holds for the case when C is invertible, resulting that $C^{-1}D$ is a symplectic matrix. Of course, even in the linear case, there are still infinitely many αs to choose from. This special case was extensively studied in [5].

4 Computation of Symplectic Maps from Generating Functions

In this section, the inverse problem is addressed. That is, given a generating function of type α, what is the symplectic map it generates? In other words, is there a "reversion" of (48) that gives $\mathcal{M}$ in terms of F and α? The answer is yes, and the algorithm is presented below.

Introduce a transformation defined by

$$T_\alpha(\mathcal{M}) = \left(\alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}\right) \circ \left(\alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix}\right)^{-1}, \tag{66}$$

where $\mathrm{Jac}(\alpha) \in Gl(4n)$, and suppose that the transversality condition is satisfied. Therefore, $T_\alpha(\mathcal{M}) = \mathcal{N}$ if and only if

$$(\mathcal{N} \circ \alpha_2 - \alpha_1) \circ \begin{pmatrix} \mathcal{M} \\ \mathcal{I} \end{pmatrix} = 0. \tag{67}$$

Now suppose that $\mathcal{M}$ is given by another transformation $T_\beta(\mathcal{K}) = \mathcal{M}$, where $\beta = (\beta_1, \beta_2)^T$, $\mathrm{Jac}(\beta) \in Gl(4n)$, with the appropriate transversality condition satisfied. Inserting it in the above equation gives

$$(\mathcal{N} \circ \alpha_2 - \alpha_1) \circ \begin{pmatrix} \left(\beta_1 \circ \begin{pmatrix} \mathcal{K} \\ \mathcal{I} \end{pmatrix}\right) \circ \left(\beta_2 \circ \begin{pmatrix} \mathcal{K} \\ \mathcal{I} \end{pmatrix}\right)^{-1} \\ \mathcal{I} \end{pmatrix} = 0. \tag{68}$$

Because $\left(\beta_2 \circ (\mathcal{K},\mathcal{I})^T\right)$ is invertible, this is equivalent to

$$(\mathcal{N} \circ \alpha_2 - \alpha_1) \circ \left(\begin{array}{c} \left(\beta_1 \circ \left(\begin{array}{c} \mathcal{K} \\ \mathcal{I} \end{array} \right)\right) \\ \left(\beta_2 \circ \left(\begin{array}{c} \mathcal{K} \\ \mathcal{I} \end{array} \right)\right) \end{array} \right) = 0, \tag{69}$$

$$(\mathcal{N} \circ (\alpha_2 \circ \beta) - (\alpha_1 \circ \beta)) \circ \left(\begin{array}{c} \mathcal{K} \\ \mathcal{I} \end{array} \right) = 0, \tag{70}$$

which in terms of T can be written as

$$T_\alpha \circ T_\beta \left(\mathcal{K}\right) = T_{\alpha \circ \beta} \left(\mathcal{K}\right), \tag{71}$$

for any $\mathcal{K}$. If we choose $\beta = \alpha^{-1}$, it follows that

$$T_\alpha \circ T_{\alpha^{-1}} = T_{\mathcal{I}} = \mathcal{I}, \tag{72}$$

that is

$$T_{\alpha^{-1}} = \left(T_\alpha\right)^{-1}. \tag{73}$$

This equation entails that whenever $T_\alpha\left(\mathcal{M}\right) = \mathcal{N}$ is well defined, the inverse is automatically well defined, and gives $\mathcal{M} = T_{\alpha^{-1}}\left(\mathcal{N}\right)$. Explicitly, this means that

$$\mathcal{M} = \left(\alpha^1 \circ \left(\begin{array}{c} \mathcal{N} \\ \mathcal{I} \end{array} \right)\right) \circ \left(\alpha^2 \circ \left(\begin{array}{c} \mathcal{N} \\ \mathcal{I} \end{array} \right)\right)^{-1}. \tag{74}$$

Applied to the situation where $\mathcal{N}$ is the gradient of the generating function and α is conformal symplectic, it gives a symplectic $\mathcal{M}$. Thus, (74) is the counterpart of (48). Together, they provide a convenient computational method to pass from F to $\mathcal{M}$ and back.

In sum, we developed the general theory of generating functions and put the results into computationally convenient forms. It has been shown that, as long as the mathematics can be performed exactly, the passing from symplectic maps to generating functions and back is easy to achieve. Moreover, this can be done utilizing any of the infinite set of generator types.

5 Transformation Properties of Generating Functions

By looking at how the generating functions transform under modifications of α and/or $\mathcal{M}$, a set of rules is obtained, which are called transformation properties. These properties are based on the fact that if α is a conformal symplectic map such that

$$\left(\mathrm{Jac}\left(\alpha\right)\right)^T J_{4n}\, \mathrm{Jac}\left(\alpha\right) = \mu \tilde{J}_{4n}, \tag{75}$$

then for any β and γ such that

$$\left(\mathrm{Jac}\left(\beta\right)\right)^T J_{4n}\, \mathrm{Jac}\left(\beta\right) = J_{4n}, \tag{76}$$

$$\left(\mathrm{Jac}\left(\gamma\right)\right)^T \tilde{J}_{4n}\, \mathrm{Jac}\left(\gamma\right) = \tilde{J}_{4n}, \tag{77}$$

the map $\beta\circ\alpha\circ\gamma$ is also a valid conformal symplectic map. Indeed, it follows from (76) and (77) and repeated application of the chain rule that $\beta\circ\alpha\circ\gamma$ satisfies (75). Therefore, it gives another type of generating function. In invariant form, if $\alpha^*\omega_0 = \mu\omega$, $\beta^*\omega_0 = \omega_0$, and $\gamma^*\omega = \omega$, then

$$(\beta\circ\alpha\circ\gamma)^*\,\omega_0 = \gamma^*\left(\alpha^*\left(\beta^*\omega_0\right)\right) = \gamma^*\left(\alpha^*\omega_0\right) = \gamma^*\left(\mu\omega\right) = \mu\omega. \tag{78}$$

These rules are interesting in their own right in symplectic geometry, and some of them can be found in [19]. The rules are used for equivalence class reduction of the set of generating functions [5].

We begin with studying what happens to the generating function $F_{\alpha,\mathcal{M}}$ under the transformation $\alpha_1 \mapsto \lambda\alpha_1$, for some non-zero real λ. This affects only the conformality factor μ of α, which becomes $\lambda\mu$. Slight rearrangement of (48) gives

$$\left(\left(\nabla F_{\alpha,\mathcal{M}}\right)^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0. \tag{79}$$

Then, we also have

$$\left(\left(\nabla F_{\begin{pmatrix}\lambda\alpha_1\\ \alpha_2\end{pmatrix},\mathcal{M}}\right)^T\circ\alpha_2-\lambda\cdot\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{80}$$

which is equivalent to

$$\left(\left(\nabla\left(\lambda^{-1}\cdot F_{\begin{pmatrix}\lambda\alpha_1\\ \alpha_2\end{pmatrix},\mathcal{M}}\right)\right)^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0. \tag{81}$$

Comparing (79) with (81) we see that

$$\nabla F_{\alpha,\mathcal{M}}=\nabla\left(\lambda^{-1}\cdot F_{\begin{pmatrix}\lambda\alpha_1\\ \alpha_2\end{pmatrix},\mathcal{M}}\right), \tag{82}$$

that is

$$F_{\begin{pmatrix}\lambda\alpha_1\\ \alpha_2\end{pmatrix},\mathcal{M}}=\lambda\cdot F_{\alpha,\mathcal{M}}+c, \tag{83}$$

for some arbitrary constant c.

In the same way, the transformation $\alpha_2\mapsto\lambda\alpha_2$ has the following effect:

$$\left(\left(\nabla F_{\begin{pmatrix}\alpha_1\\ \lambda\alpha_2\end{pmatrix},\mathcal{M}}\right)^T\circ(\lambda\cdot\alpha_2)-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{84}$$

$$\left(\left(\left(\nabla F_{\begin{pmatrix}\alpha_1\\ \lambda\alpha_2\end{pmatrix},\mathcal{M}}\right)^T\circ\lambda\mathcal{I}\right)\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{85}$$

$$\left(\lambda^{-1}\cdot\left(\nabla\left(F_{\begin{pmatrix}\alpha_1\\ \lambda\alpha_2\end{pmatrix},\mathcal{M}}\circ\lambda\mathcal{I}\right)\right)^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{86}$$

$$\left(\left(\nabla\left(\lambda^{-1}\cdot\left(F_{\begin{pmatrix}\alpha_1\\ \lambda\alpha_2\end{pmatrix},\mathcal{M}}\circ\lambda\mathcal{I}\right)\right)\right)^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0. \tag{87}$$

Again, comparison of (79) and (87) gives

$$\nabla\left(\lambda^{-1}\cdot\left(F_{\left(\begin{smallmatrix}\alpha_1\\ \lambda\alpha_2\end{smallmatrix}\right),\mathcal{M}}\circ\lambda\mathcal{I}\right)\right)=\nabla F_{\alpha,\mathcal{M}}, \tag{88}$$

that is

$$F_{\left(\begin{smallmatrix}\alpha_1\\ \lambda\alpha_2\end{smallmatrix}\right),\mathcal{M}}=\lambda\cdot F_{\alpha,\mathcal{M}}\circ\lambda^{-1}\mathcal{I}+c. \tag{89}$$

Also, from these two transformation properties it is easy to see the effect of the two transformations combined.

Next, we study what happens if we change the symplectic map, for example, by $\mathcal{M}\mapsto\mathcal{M}\circ\mathcal{A}$, for some symplectic map $\mathcal{A}$. From (48) we have

$$\left((\nabla F_{\alpha,\mathcal{M}\circ\mathcal{A}})^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\circ\mathcal{A}\\ \mathcal{I}\end{pmatrix}=0 \tag{90}$$

$$\left((\nabla F_{\alpha,\mathcal{M}\circ\mathcal{A}})^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{A}^{-1}\end{pmatrix}=0 \tag{91}$$

$$\left((\nabla F_{\alpha,\mathcal{M}\circ\mathcal{A}})^T\circ(\alpha_2\circ T_{\mathcal{A}})-(\alpha_1\circ T_{\mathcal{A}})\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{92}$$

where $T_{\mathcal{A}}$ is defined by $T_{\mathcal{A}}(\hat{z},z)=\left(\hat{z},\mathcal{A}^{-1}(z)\right)$. Equation (92) can be written also as

$$\left((\nabla F_{\alpha\circ T_{\mathcal{A}},\mathcal{M}})^T\circ(\alpha_2\circ T_{\mathcal{A}})-(\alpha_1\circ T_{\mathcal{A}})\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{93}$$

from where we conclude

$$F_{\alpha,\mathcal{M}\circ\mathcal{A}}=F_{\alpha\circ T_{\mathcal{A}},\mathcal{M}}+c. \tag{94}$$

In the same manner, the left action of another symplectomorphism on the map, i.e. $\mathcal{M}\mapsto\mathcal{K}\circ\mathcal{M}$ leads to

$$\left((\nabla F_{\alpha,\mathcal{K}\circ\mathcal{M}})^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{K}\circ\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0. \tag{95}$$

Define $T_{\mathcal{K}}(\hat{z},z)=(\mathcal{K}(\hat{z}),z)$. Then,

$$F_{\alpha,\mathcal{K}\circ\mathcal{M}}=F_{\alpha\circ T_{\mathcal{K}},\mathcal{M}}+c. \tag{96}$$

We are also interested what happens when we change the coordinates in the generating function, $F\mapsto F\circ\mathcal{L}$, by a diffeomorphism $\mathcal{L}$ (here not necessarily a symplectomorphism); we have

$$\left((\nabla(F\circ\mathcal{L}))^T\circ\alpha_2-\alpha_1\right)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0 \tag{97}$$

$$(\mathrm{Jac}(\mathcal{L}))^T\cdot\left(\nabla F\right)^T\circ\mathcal{L}\circ\alpha_2-\alpha_1)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0 \tag{98}$$

$$\left(\nabla F_{T_{\mathcal{L}}\circ\alpha,\mathcal{M}}\right)^T\circ(\mathcal{L}\circ\alpha_2)-\left((\mathrm{Jac}(\mathcal{L}))^{-T}\cdot\alpha_1\right)\Big)\circ\begin{pmatrix}\mathcal{M}\\ \mathcal{I}\end{pmatrix}=0, \tag{99}$$

where we defined $T_{\mathcal{L}}(\hat{z}, z) = \left((\text{Jac}(\mathcal{L}))^{-T} \cdot \hat{z}, \mathcal{L}(z)\right)$. Hence,

$$\nabla \left(F_{T_{\mathcal{L}} \circ \alpha, \mathcal{M}} \circ \mathcal{L}\right) = \nabla F_{\alpha, \mathcal{M}}, \tag{100}$$

that is

$$F_{T_{\mathcal{L}} \circ \alpha, \mathcal{M}} = F_{\alpha, \mathcal{M}} \circ \mathcal{L}^{-1} + c. \tag{101}$$

Finally, if we replace $\mathcal{M}$ with $\mathcal{M}^{-1}$, we arrive to

$$\left(\left(\nabla F_{\alpha, \mathcal{M}^{-1}}\right)^T \circ \alpha_2 - \alpha_1\right) \circ \begin{pmatrix} \mathcal{M}^{-1} \\ \mathcal{I} \end{pmatrix} = 0. \tag{102}$$

Applying $\mathcal{M}$ from the right we get

$$\left(\left(\nabla F_{\alpha, \mathcal{M}^{-1}}\right)^T \circ \alpha_2 - \alpha_1\right) \circ \begin{pmatrix} \mathcal{I} \\ \mathcal{M} \end{pmatrix} = 0. \tag{103}$$

This is equivalent to say that, if in both α_1 and α_2 we interchange the first $2n$ variables with the second $2n$, we get back $F_{\mathcal{M}}$ with this changed α. In terms of the Jacobian $\alpha_\#$, or in case of linear αs, this can be written as the transformation

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \mapsto \begin{pmatrix} B & A \\ D & C \end{pmatrix}, \tag{104}$$

so we can conclude that

$$F_{\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right), \mathcal{M}^{-1}} = F_{\left(\begin{smallmatrix} B & A \\ D & C \end{smallmatrix}\right), \mathcal{M}} + c. \tag{105}$$

6 Summary

The extended theory of generating functions of canonical transformations was developed. Using a modified definition of the generating function, it was showed that there are many more generating functions than commonly known, and some always are defined globally. Throughout, methods of symplectic geometry have been utilized. In the appropriate language, both symplectic maps and generating functions are the same geometrical objects, namely Lagrangian submanifolds. The type of the generating function is determined by the identification diffeomorphisms, which turn out to be restrictions of local conformal symplectomorphisms. We showed how the geometric theory can be cast into a convenient computational framework, and derived a variety of transformation rules for generating functions. For the interested reader, various applications can be found in [5, 20, 21]. The results of this paper will also be applied in further developing the theory of optimal symplectification according to [4].

References

[1] H. Goldstein. *Classical Mechanics*. Addison-Wesley, Reading, MA, 1980.

[2] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration.* Springer, 2002.

[3] M.L. Shashikant, M. Berz, and B. Erdelyi. COSY Infinity's EXPO Symplectic Tracking for LHC. *Inst. of Physics CS*, 175:299–306, 2004.

[4] B. Erdelyi and M. Berz. Optimal symplectic approximation of Hamiltonian flows. *Phys. Rev. Lett.*, 87 (11):114302, 2001.

[5] B. Erdelyi and M. Berz. Local theory and applications of extended generating functions. *Int. J. of Pure and Applied Mathematics*, 11 (3):241–282, 2004.

[6] M. Berz. *Modern Map Methods in Particle Beam Physics.* Academic Press, San Diego, 1999, also available at http://bt.nscl.msu.edu/paperscgi/display.pl ?name=AIEP108book.

[7] Henri Poincare. *New Methods of Celestial Mechanics*, volume 3, chap. XXVIII. American Institute of Physics, New York, 1893/1993.

[8] A. Weinstein. The invariance of Poincare's generating function for canonical transformations. *Invent. Math.*, 16:203–213, 1972.

[9] K. Feng, H.M. Wu, M.Z. Quin, and D.L. Wang. Construction of canonical difference schemes for Hamiltonian formalism via generating functions. *J. Comp. Math.*, 7, 1:71–96, 1989.

[10] D. McDuff and D. Salamon. *Introduction to symplectic topology.* Oxford University Press, New York, 1995.

[11] H. Hofer and E. Zehnder. *Symplectic invariants and Hamiltonian dynamics.* Birkhauser, Basel, 1994.

[12] A. Banyaga. *The structure of classical diffeomorphism groups.* Dordrecht, Boston, Kluwer Academic, 1997.

[13] J. E. Marsden and T. S. Ratiu. *Introduction to Mechanics and Symmetry.* Springer-Verlag, New York, 1994.

[14] A. Weinstein. Lagrangian submanifolds and Hamiltonian systems. *Ann. of Math.*, 98, 2:377–410, 1973.

[15] A. Weinstein. Symplectic manifolds and their Lagrangian submanifolds. *Advances in Math.*, 6:329–346, 1971.

[16] P. Libermann and C.M. Marle. *Symplectic geometry and analytical mechanics.* Dordrecht, Boston, Kluwer Academic, 1987.

[17] I. Vaisman. *Symplectic geometry and secondary characteristic classes.* Prog. in Math., Birkhauser, Boston, 1987.

[18] M. Gromov. Pseudo-holomorphic curves in symplectic manifolds. *Invent. Math.*, 82:307–347, 1985.

[19] K. Feng. The calculus of generating functions and the formal energy for Hamiltonian algorithms. *J. Comp. Math.*, 16, 6:481–498, 1998.

[20] B. Erdelyi and M. Berz. Optimal generating function symplectification of order-by-order symplectic Taylor maps. In *Proceedings of the 6th International Computational Accelerator Physics Conference*, Darmstadt, Germany, http://130.83.124.174/frames/index.htm, 2000. TU Darmstadt.

[21] B. Erdelyi, J. Hoefkens, and M. Berz. Rigorous lower bounds for the domains of definition of extended generating functions. *SIAM J. on Aplied Dynamical Systems*, accepted, 2005.