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Anatomy of the canonical transformation

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A concise account of the structure of the canonical transformation is given, in the lowest dimensional case. This case is chosen because it offers a special clarity in several respects. In particular, the diversity of possible generating functions is illustrated by many examples which are not available elsewhere. Many of these are of physical interest, and some of them are multivalued. These examples are used to inform a comparative study of the several different definitions of a canonical transformation to be found in the literature.

The paper is pertinent to all those branches of mechanics which can be given a hamiltonian representation. These include not only the classical dynamics of particles and rigid bodies, but also some more recent studies in continuum mechanics, including geophysical fluid dynamics.

An area of particular modern interest is that of symplectic integrators. These are numerical integrating algorithms which generate a solution to Hamilton's equations via a sequence of canonical transformations, which preserve the hamiltonian structure in the numerical solution.

1. Introduction

The aim of this paper is to conduct a fresh study of the canonical transformation. This transformation is widely known to be a classical and time-honoured device in mechanics, but we have found that the standard texts often treat it in a way which is either stereotyped and rather uncritical, or sophisticated and unduly difficult. Understanding of it may be no more than formal without a reasonable variety of explicit examples. The literature seems not to offer the variety which we have in mind, and one of the purposes of this paper is to provide such examples.

The anatomy of a canonical transformation is revealed in the different ways by which it can be expressed as the gradients of generating functions. Our examples seek to bring out some attractive aspects which we have not seen elsewhere, and they illustrate the mathematical and physical diversity of possible generating functions.

The importance of the canonical transformation derives from the fact that it is intrinsic in any part of mathematics or mechanics where Hamilton's equations may appear. Arnold (1989, p. 233) remarks that the technique of generating functions, developed by Hamilton and Jacobi, is the most powerful method available for integrating the differential equations of dynamics. As we indicate in §3, a canonical transformation leaves the structure of Hamilton's equations invariant.

In recent years there has been a resurgence of interest in Hamilton's equations, with particular reference to the computation of numerical solutions of them, and this part of the literature has been reviewed by Sanz-Serna (1992). Numerical integrating

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algorithms generate a solution to Hamilton's equations via a sequence of coordinate transformations. If the latter are canonical (sometimes called symplectic), then the numerical solutions will inherit the structural invariance present in Hamilton's equations. Algorithms with such a property are often called symplectic integrators, and we give an example in §5*d*.

The more recent adjective 'symplectic' is tending to take over from the classical one 'canonical'. For the purposes of this paper we can regard them as synonymous. Further elaboration of the definition of 'symplectic' is given by Marsden (1992, p. 10) and Sanz-Serna (1992, §§2–5).

The trigger for the present paper lay within our investigation of the semi-geostrophic equations of meteorology. Previous papers (Chynoweth & Sewell 1989, 1990, 1991) showed that topic to contain convexifications of multivalued Legendre dual functions such as the swallowtail, which are adapted here to provide examples of canonical transformations. That work itself grew from the representation of an atmospheric front as a crease in a single-valued surface, whose gradients are temperature and velocity, which therefore jump across the crease, and from associated numerical solutions (Purser & Cullen 1987; Chynoweth 1987).

It is quite common for discussion of canonical transformations to be phrased in terms of differentials. A differential is a local device, and carries an implication of single valuedness if ambiguity is to be avoided. A differential may also fail to warn that the degree of freedom within the implied domain is restricted. Our examples will show that generating functions can often be multivalued globally, and that their definition is sometimes necessarily restricted to a domain of lower dimension than might be suggested by an equation expressed in terms of differentials. For these reasons, differentials do not figure prominently in this paper, except in certain comments on other work. Instead, our viewpoint is to emphasize the generating functions themselves, and their derivatives.

2. Definition

The choice of definition for a canonical transformation is evidently a matter of taste, because at least five definitions can be found in the literature. These are not all equivalent, as we shall explain.

It is clearest to deal with the lowest dimensional case, because this offers fully explicit examples in a way which higher dimensions, for all their importance, cannot. We use a neutral notation, as does Carathéodory (1982) for example, which is not biased towards any particular context. Thus we suppose that a pair x, y of real scalars is related to another such pair X, Y by

$$X = X(x, y), \quad Y = Y(x, y). \tag{1}$$

The expressions on the right are two differentiable functions, and we have used the same symbol for a function and its values. Thus (1) is a dependence or transformation $R^2 \rightarrow R^2$.

Let

$$j = \frac{\partial X}{\partial x}\frac{\partial Y}{\partial y} - \frac{\partial X}{\partial y}\frac{\partial Y}{\partial x}$$

denote the jacobian of (1). In general, j will also be a function $j(x, y)$ of x and y. For some particular transformations (1), however, this function has a constant value over some domain in x, y space.

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We adopt the following definition for the purposes of this paper. If the transformation (1) has

$$j = 1 \tag{2}$$

over a two-dimensional domain, we define the transformation to be *canonical over that domain*. The domain need not be the whole space.

Carathéodory (1982, p. 79) says that Jacobi was the first to consider canonical transformations, and that Poincaré used the following example in celestial mechanics. If c and k are constants the transformation

$$X = x^c \cos 2ky, \quad Y = x^c \sin 2ky$$

has $j = 2ckx^{2c-1}$. Thus if $c = \frac{1}{2}$, j is the constant k over $x \geqslant 0$, and $j = 1$ if $k = 1$. Therefore

$$X = x^{\frac{1}{2}} \cos 2y, \quad Y = x^{\frac{1}{2}} \sin 2y \tag{3}$$

is a canonical transformation over the half-plane $x \geqslant 0$.

Theorem 1. *If k is a non-zero constant such that $j = k$ over some domain, then we may choose $k = 1$ without loss of generality.*

Proof. If $k > 0$, the transformation can be rescaled by multiplying X and Y each by $k^{-\frac{1}{2}}$, which has the effect of replacing k by 1.

If $k < 0$, the transformation can be rescaled by multiplying X by $-(-k)^{-\frac{1}{2}}$ and Y by $(-k)^{-\frac{1}{2}}$, or vice versa, which again has the effect of replacing k by 1. □

This theorem means that a canonical transformation is available whenever $j = k \neq 0$, just by rescaling of variables. The above example with $c = \frac{1}{2}$ provides an illustration. Evidently such rescaling cannot be performed if $k = 0$.

Another simple example of a canonical transformation is

$$X = x, \quad Y = x^2 + y. \tag{4}$$

We shall see in figure 2 how this contains hidden features of modern interest.

3. Motivation

Hamilton's equations are

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{\partial h}{\partial y}, \quad \frac{\mathrm{d}y}{\mathrm{d}t} = \frac{\partial h}{\partial x}, \tag{5}$$

where the function $h(x, y, t)$ is the hamiltonian and t is time. The transformation (1) implies, by the chain rule without using (2), that (5) have the properties

$$\frac{\mathrm{d}X}{\mathrm{d}t} = -j\frac{\partial H}{\partial Y}, \quad \frac{\mathrm{d}Y}{\mathrm{d}t} = j\frac{\partial H}{\partial X},$$

where $H(X, Y, t) = h(x, y, t)$ denotes the original hamiltonian expressed in terms of the new variables.

Therefore a canonical transformation leaves invariant both the form of Hamilton's equations and the value of the hamiltonian function, by (2). This is the straightforward historical motivation for interest in the canonical transformation. We have mentioned the role of symplectic integrators in §1.

The transcriptions, $x, y, X, Y \leftrightarrow p, q, P, Q$, respectively, to notation which Lanczos (1949, p. 196) attributes to Whittaker (1937, §126), serve as a reminder of

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applications in classical mechanics, with generalized coordinate q and momentum p. Then it is said that (2) expresses incompressibility of the so-called phase space under a canonical transformation.

Another motivation for studying canonical transformations is the importance of incompressible plane deformations in continuum mechanics, although the connection between the two topics is not normally exploited in either field. Water, air up to a certain speed, rubber as an elastic solid, and metal in plastic distortion, are often treated as incompressible media. The adjective 'canonical' is not usually used by authors in this field, 'isochoric' being preferred by some (see, for example, Truesdell & Toupin 1960, §40), also for a three dimensional incompressible deformation. If x, y are the cartesian coordinates of a typical particle before deformation, and X, Y are its cartesian coordinates afterwards, equations (1) describe the deformation, which is incompressible if (2) holds. An example is provided by the most general homogeneous plane deformation,

$$X = ax+hy+g, \quad Y = cx+by+f,$$

in which a, h, g, c, b, f are constants, so that $j = ab-hc$. This is incompressible if $j = 1$. Simple shear is a specific example, in which $a = b = 1$, $c = g = f = 0$ and $h \neq 0$. If the coordinates in (3) are cartesian, it describes a non-homogeneous deformation which is the bending of a rectangular block such as $0 < a \leqslant x \leqslant b$, $|y| \leqslant c < \frac{1}{4}\pi$ into part of a circular annulus with $a^{\frac{1}{2}}$ and $b^{\frac{1}{2}}$ as internal and external radii, and with straight radial ends subtending an angle $4c$, where a, b, c are constants. This example, with others, appears in many texts on finite elasticity, such as Green & Adkins (1960) and Ogden (1984). Complex variable methods are used in that field, and in fluid mechanics.

The cartesian components u, v of the plane velocity of a particle with cartesian position coordinates x, y are expressible as

$$u = -\partial\psi/\partial y, \quad v = \partial\psi/\partial x \tag{6}$$

in terms of a stream function $\psi(x, y, t)$ of x, y and time t, when the medium is incompressible. After a small time ϵ the new cartesian coordinates of the particle are approximately

$$X = x-\epsilon\,\partial\psi/\partial y, \quad Y = y+\epsilon\,\partial\psi/\partial x.$$

This illustrates what is known as an *infinitesimal canonical transformation* (see Arnold 1989, §48C), in the sense that $j = 1+O(\epsilon^2)$. A specific example is provided by steady flow past a circular cylinder of radius a, for which

$$\psi = cy(a^2/(x^2+y^2)-1) \tag{7}$$

when the stream has speed c at infinity in the direction of the x-axis. An infinitesimal canonical transformation is only an approximation to a true canonical transformation. To obtain the latter in incompressible fluid mechanics, one must integrate the motion to express the spatial (eulerian) coordinates in terms of the material (lagrangian) coordinates.

In these ways the kinematics of plane incompressible media offer many examples of canonical transformations.

4. Anatomy

We return to the neutral general notation of §2. A canonical transformation has a locally unique inverse in the neighbourhood of every point of its domain, because $j = 1$ is sufficient for the inverse function theorem to apply (see Apostol 1974, Theorem 13.6). Even when the functions in (1) are single valued, however, the global inverse of the transformation, which we write as

$$x = x(X, Y), \quad y = y(X, Y) \tag{8}$$

in terms of differentiable functions on the right, need not be single valued. An example is the inverse of (3), which is

$$x = X^2 + Y^2, \quad y = \tfrac{1}{2} \arctan Y/X. \tag{9}$$

We must restrict the domain of (3) to a principal half-strip such as $x \geqslant 0$, $|y| < \frac{1}{4}\pi$ to ensure that (9) is also single valued globally. The domain of (9) is then the half-plane $X \geqslant 0$, all Y.

Such global multivaluedness of the inverse can be more elaborate in its details in other cases, such as Examples 2 and 3 of Whittaker (1937, §126).

Aside from this type of complication, however, the canonical transformation is a bland device in the sense of being always non-singular. We define a singularity of (1) to be a location in the x, y plane where $j = 0$ or $\pm\infty$.

This bland exterior conceals some variety of anatomical detail within the canonical transformation which we now seek to explore. It is convenient to define an *internal singularity* of a canonical transformation to be a location where one or more of $\partial X/\partial x$, $\partial X/\partial y$, $\partial Y/\partial x$, $\partial Y/\partial y$ is zero or infinite. These often occur even though $j = 1$, and we have to allow for that. For (3) over the principal half-strip, internal singularities are isolated along $x = 0$ and along $y = 0$. For (4) $\partial Y/\partial x = 0$ along $x = 0$, but $\partial X/\partial y \equiv 0$.

Theorem 2. *A canonical transformation* (1) *with* (2) *can be expressed locally in one or more of the following versions, when the indicated sufficient condition holds.*

(i) *If* $\partial Y/\partial y \neq 0, \pm\infty$, *then* $X = X(x, Y)$, $y = y(x, Y)$ *such that*

$$\partial X/\partial x = \partial y/\partial Y. \tag{10}$$

(ii) *If* $\partial X/\partial y \neq 0, \pm\infty$, *then* $y = y(x, X)$, $Y = Y(x, X)$ *such that*

$$\partial y/\partial X + \partial Y/\partial x = 0. \tag{11}$$

(iii) *If* $\partial X/\partial x \neq 0, \pm\infty$, *then* $x = x(X, y)$, $Y = Y(X, y)$ *such that*

$$\partial x/\partial X = \partial Y/\partial y. \tag{12}$$

(iv) *If* $\partial Y/\partial x \neq 0, \pm\infty$, *then* $X = X(Y, y)$, $x = x(Y, y)$ *such that*

$$\partial X/\partial y + \partial x/\partial Y = 0. \tag{13}$$

Proof. Suppose that $\partial Y/\partial y \neq 0, \pm\infty$. Then $(1)_2$ can be inverted as $y = y(x, Y)$ uniquely locally in (10), and substituted into $(1)_1$ to give the new function $X(x, Y) = X(x, y(x, Y))$ in terms of the old function $X(x, y)$. The chain rule applied to new and old functions gives

$$\frac{\partial X}{\partial x} = \frac{\partial X}{\partial x} + \frac{\partial X}{\partial y}\frac{\partial y}{\partial x} \quad \text{with} \quad 0 = \frac{\partial Y}{\partial x} + \frac{\partial Y}{\partial y}\frac{\partial y}{\partial x}, \quad 1 = \frac{\partial Y}{\partial y}\frac{\partial y}{\partial Y}$$

so that
$$\frac{\partial X}{\partial x} = \frac{\partial X}{\partial x} - \frac{\partial X}{\partial y}\frac{\partial Y}{\partial x}\bigg/\frac{\partial Y}{\partial y} = j\frac{\partial y}{\partial Y}.$$

Now using (2) gives the last equation in (10).

Similar reasoning leads to (11), (12) and (13). □

There may be locations where not all of the hypotheses in (i)–(iv) hold, and yet $j=1$.

There might also be locations where none of the hypotheses in (i)–(iv) hold, and yet still $j=1$. For example, it could happen that $\partial X/\partial x=0$, $\partial Y/\partial y=\infty$, $\partial X/\partial y=0$, $\partial Y/\partial x=\infty$, all such that $j=1$.

In thermodynamics, the last equations in (10)–(13) are called Maxwell's relations, an example which we give in §5*c*.

Theorem 3. *For each part of Theorem 2 which is available, there exists a scalar* generating function *listed below, allowing the canonical transformation to be expressed in gradient form as follows, and locally so in the first instance.*

(i) $A(x,Y)$ *such that*

$$X=\partial A/\partial Y, \quad y=\partial A/\partial x. \tag{14}$$

(ii) $B(x,X)$ *such that*

$$y=-\partial B/\partial x, \quad Y=\partial B/\partial X. \tag{15}$$

(iii) $C(X,y)$ *such that*

$$x=-\partial C/\partial y, \quad Y=-\partial C/\partial X. \tag{16}$$

(iv) $D(Y,y)$ *such that*

$$X=-\partial D/\partial Y, \quad x=\partial D/\partial y. \tag{17}$$

Proof. The last conditions in (10)–(13) are integrability conditions which are, respectively, necessary and sufficient for the properties (14)–(17). □

The generating functions in Theorem 3 are available locally and as single-valued functions in the first instance, but we shall give examples showing how they can be available globally, and as multivalued functions, capable of self-intersection such as figure 5 illustrates in particular. The idea of generating functions is well known in the literature on classical mechanics (see Goldstein 1950, ch. 8; Synge 1960, §88), but the variety of their possible forms which we shall indicate here is not.

It can be shown that a time-dependent canonical transformation preserves the form of Hamilton's equations provided the value of the hamiltonian function is augmented by the partial time derivative of a generating function.

Theorem 4. *When any two of the generating functions having one argument in common exist, they are connected by a Legendre transformation which relates the non-common arguments as active variables, while the common one is passive.*

Proof. Suppose that (1) has the properties

$$\partial Y/\partial y \neq 0, \pm\infty \quad \text{and} \quad \partial X/\partial y \neq 0, \pm\infty. \tag{18}$$

These are sufficient for (14) and (15) to apply locally, by Theorems 2 and 3. We recognize there the standard form of mutual inverses

$$X=\partial A/\partial Y=X(x,Y), \quad Y=\partial B/\partial X=Y(x,X)$$

expressible via a non-singular Legendre transformation whose dual functions $A(x,Y)$ and $B(x,X)$ are related by

$$A+B=YX \quad \text{and} \quad \partial A/\partial x+\partial B/\partial x=0. \tag{19}$$

That (18) are sufficient to justify the inversion between the dual active variables is confirmed by

$$\frac{\partial X}{\partial Y}=\frac{\partial X/\partial y}{\partial Y/\partial y}\neq 0, \pm\infty.$$

Gradients of the functions (1) are on the right here, and of $X(x,Y)$ on the left.

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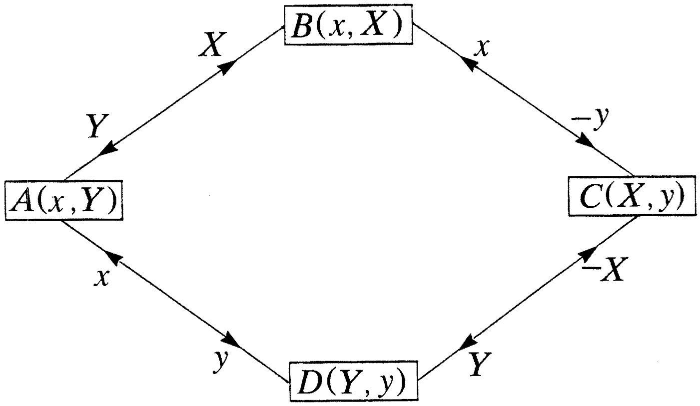

Figure 1. Quartet of Legendre transformations.

A similar argument applies when the three other pairs (15)+(16), (16)+(17), and (17)+(14) are available in turn. □

Theorem 5. *When all four of the generating functions in Theorem* 3 *exist, they are related by the closed quartet of Legendre transformations represented mnemonically by figure* 1, *and analytically in* (20). *Each pair of functions is connected by a line representing a Legendre transformation whose active variables, participating in the gradients of the respective functions, are written next to the arrows on that line. The sum of the functions is equal to the product of the active variables. That is,*

$$\left.\begin{array}{lll} A+B=XY, & X=\partial A/\partial Y, & Y=\partial B/\partial X, \\ B+C=-xy, & x=-\partial C/\partial y, & y=-\partial B/\partial x, \\ C+D=-XY, & X=-\partial D/\partial Y, & Y=-\partial C/\partial X, \\ D+A=xy, & x=\partial D/\partial y, & y=\partial A/\partial x. \end{array}\right\} \tag{20}$$

Proof. The result is a résumé of (14), (15), (19) and their counterparts. □

Figure 1 is another example of a general scheme explained by Sewell (1987, fig. 2.18) for closed chains of Legendre transformations connecting scalar functions of $n+m$ variables. Here $n=m=1$. Particular examples of such quartets in the mechanics of solids and fluids are given by Sewell (1987), and in meteorology by Chynoweth & Sewell (1989, 1991). The local shapes of the functions are related: e.g. if D is jointly convex so is $-B$, and then A and C are complementary saddle functions.

The globally valid functions which generate our first example (3) of a canonical transformation are as follows. We treat the power $\frac{1}{2}$ as designating only the positive square root, so that (3) is single valued over $x \geqslant 0$. To ensure that (9) is single valued we consider only $|y| < \frac{1}{4}\pi$. Then

$$\left.\begin{array}{llll} A(x,Y)=\frac{1}{2}x \arcsin Y/x^{\frac{1}{2}}+\frac{1}{2}Y(x-Y^2)^{\frac{1}{2}} & \text{over} & x \geqslant Y^2, & \text{all } Y, \\ B(x,X)=-\frac{1}{2}x \arccos X/x^{\frac{1}{2}} \pm \frac{1}{2}X(x-X^2)^{\frac{1}{2}} & \text{over} & x \geqslant X^2, & X \geqslant 0, \\ C(X,y)=-\frac{1}{2}X^2 \tan 2y & \text{over} & |y|<\frac{1}{4}\pi, & X \geqslant 0, \\ D(Y,y)=-\frac{1}{2}Y^2 \cot 2y & \text{over} & |y|<\frac{1}{4}\pi, & \text{all } Y. \end{array}\right\} \tag{21}$$

It is convenient to derive $D(Y,y)$ first, by integration of $(17)_2$ after inverting $(3)_2$ as

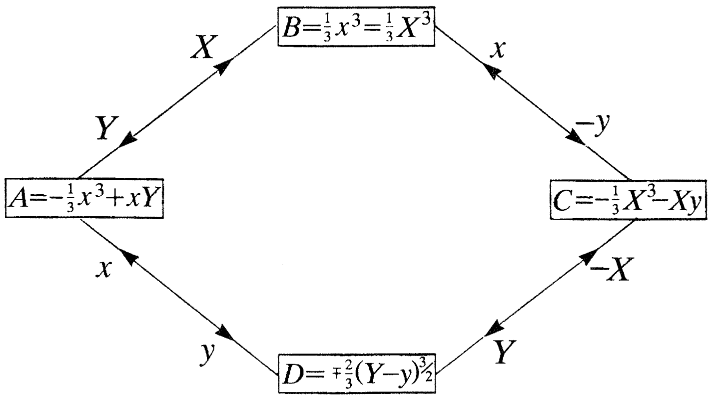

Figure 2. Legendre quartet for $X = x$, $Y = x^2 + y$.

$x^{\frac{1}{2}} = Y/\sin 2y$. The fact that $\partial Y/\partial x = \frac{1}{2}x^{-\frac{1}{2}}\sin 2y$ shows that there is an internal singularity at $x = 0$ and at $y = 0$, and the latter manifests itself in the infinite jump in $D(Y, 0)$. To find the other three functions requires no more integration, but just the first column of (20) in conjunction with appropriate inversions of $(3)_1$ or $(3)_2$. Evidently $C(X, y)$ and $A(x, Y)$ are also single valued, but $B(x, X)$ is double valued because we have used the inversion of $\cos 2y = X/x^{\frac{1}{2}}$ in $|y| < \frac{1}{4}\pi$. This is shown by the three vertical sections $x = \text{const.}$ in figure 3*a* which join the line $X = 0$, $B = -\frac{1}{4}\pi x$ to a vertical tangent plane where $x = X^2$, $B = 0$. Curiously, Carathéodory (1982, p. 79) gives the value $\frac{1}{4}x \sin 4y - xy$ of B in terms of x and y, but not the generating function $B(x, X)$ itself, which is the real point of (15).

The only internal singularities in the foregoing example are isolated, along $x = 0$ and along $y = 0$. The hypotheses of Theorems 2 and 3 fail there; but those hypotheses are only sufficient, and not necessary, for the inverse function theorem to hold. The example shows how, in a specific case, the construction of globally valid generating functions may not be inhibited by isolated internal singularities.

The quartet of Legendre transformations which reveal the anatomy of the canonical transformation (4) are summarized in figure 2. There are no internal singularities associated with $\partial X/\partial x = 1$ and $\partial Y/\partial y = 1$, so (14) and (16) with (4) can each be integrated to give the generating functions A and C stated in figure 2, over the whole x, Y and X, y planes respectively. These two functions each have the form of the fold catastrophe potential in its simplest cubic version. The internal singularity of $\partial Y/\partial x = 0$ at $x = 0$ is an isolated singularity of each of the lower two Legendre transformations $(20)_3$ and $(20)_4$ in figure 2, but this does not inhibit the construction of the double-valued function $D = \mp\frac{2}{3}(Y-y)^{\frac{3}{2}}$ with cusped edge of regression along $Y = y$ illustrated in figure 3*b*. This has a horizontal tangent plane where $Y = y$, by contrast with the vertical tangent plane of $B(x, X)$ where $x = X^2$ in the previous example. The form of figure 3*b* is also the bifurcation set of the cusp catastrophe potential

$$V(\xi) = \tfrac{1}{12}\xi^4 - \tfrac{1}{2}(Y-y)\,\xi^2 + D\xi,$$

where ξ is a dummy variable. The bifurcation set in the D, $Y-y$ parameter space of this function is defined by eliminating ξ from $\partial V/\partial \xi = \partial^2 V/\partial \xi^2 = 0$. It is shown by Sewell (1987, §2.3) that this bifurcation set is the Legendre dual of the fold catastrophe potential derived above in A and C, and that this result is part of a general 'ladder for the cuspoids'.

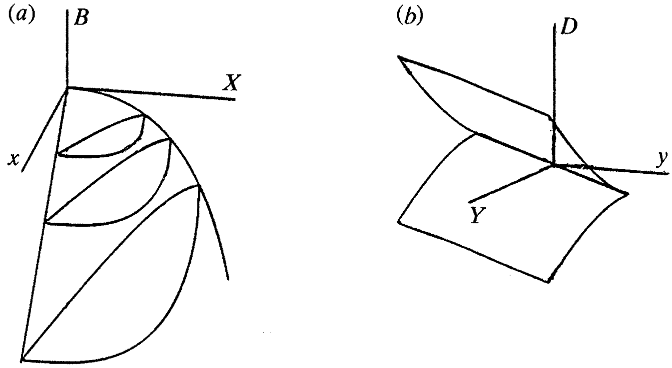

Figure 3. (*a*) $B(x, X)$ of $(21)_2$; (*b*) $D(Y, y) = \mp\frac{2}{3}(Y-y)^{\frac{3}{2}}$.

The internal singularity $\partial X/\partial y \equiv 0$ of (4) is not an isolated singularity, so that the inverse function theorem cannot be resurrected in the way that is possible for the foregoing isolated singularities. Parts (ii) of Theorems 2 and 3 fail in the stated forms. Nevertheless, the upper two Legendre transformations in figure 2 can still be reconstructed by using the more basic definition of a Legendre transformation in terms of poles and polars (see Sewell 1987, §2.2). Each of $A(x, Y)$ and $C(X, y)$ is linear in the variable now required to be active, namely Y and y respectively, and the dual of these polars is the single point, with abscissa $x = X$ and ordinate $\frac{1}{3}x^3 = \frac{1}{3}X^3$, read off from the first two equations of $(20)_1$ and $(20)_2$, which do survive. The generating function $B(x, X)$ still exists, therefore, but only over a domain of lower dimension (one instead of two), and so must be handled appropriately. One may not know in advance which generating functions have this limitation.

This means, for example, that care is required if differentials are used. For example, although $\mathrm{d}A = y\mathrm{d}x + X\mathrm{d}Y$ can be rewritten as $\mathrm{d}B = -y\mathrm{d}x + Y\mathrm{d}X$ with $B = XY - A$, we cannot infer (15) because x and X are not independent. We avoid differentials in this paper except in (51), (52), (55) and (56), preferring a more explicit description in terms of functions themselves.

The foregoing properties of the example (4) of a canonical transformation can be generalized in the following direction.

Theorem 6. *The most general canonical transformation in which X is a function $X(x)$ independent of y and having finite non-zero slope $\mathrm{d}X/\mathrm{d}x$ must be of the form*

$$X = X(x), \quad Y = \left(y + \frac{\mathrm{d}\beta}{\mathrm{d}x}\right) \bigg/ \frac{\mathrm{d}X}{\mathrm{d}x} \tag{22}$$

at least locally, where $\beta(x)$ is an arbitrary differentiable function.

Proof. The hypothesis of part (iii) of Theorems 2 and 3 holds, so $C(X, y)$ exists such that $\partial C/\partial y = -x(X)$, where $x(X)$ is the single-valued local inverse of $X(x)$. Integrating gives $C(X, y) = -yx(X) - b(X)$, where $b(X)$ is an arbitrary function of X. From $(16)_3$

$$Y = y\frac{\mathrm{d}x}{\mathrm{d}X} + \frac{\mathrm{d}b}{\mathrm{d}X} = \left(y + \frac{\mathrm{d}\beta}{\mathrm{d}x}\right) \bigg/ \frac{\mathrm{d}X}{\mathrm{d}x}.$$

Here $\beta(x) = b(X(x))$ is an arbitrary function of x, having the values of the generating function $B(x, X)$ which is defined only on the curve $X = X(x)$ in the x, X plane. □

Thus the second function in (1) must be linear in y if the first does not contain y and the transformation is to be canonical.

Then $\partial Y/\partial y = \mathrm{d}x/\mathrm{d}X$ is also finite and non-zero, so that

$$A(x,Y) = YX(x) - \beta(x)$$

exists satisfying (14) and the first of (20). For $D(Y,y)$ to exist it is sufficient that

$$\left(\frac{\mathrm{d}X}{\mathrm{d}x}\right)^2 \frac{\partial Y}{\partial x} = \frac{\mathrm{d}X}{\mathrm{d}x}\frac{\mathrm{d}^2\beta}{\mathrm{d}x^2} - \left(y + \frac{\mathrm{d}\beta}{\mathrm{d}x}\right)\frac{\mathrm{d}^2X}{\mathrm{d}x^2}$$

be finite and non-zero. The values of D are those of

$$D = xy - XY + \beta.$$

For example, if $X = x$ and $\beta = (2n+1)^{-1}x^{2n+1}$ with positive integral n, then

$$Y = y + x^{2n} \quad \text{and} \quad D = \mp [2n/(2n+1)](Y-y)^{(2n+1)/2n}.$$

We have $n = 1$ in (4) and figure 3*b*.

Another example of some particular interest occurs if β is a constant, or $\beta = 0$ without loss of generality. Then $(22)_2$ is homogeneous linear in y (cf. Carathéodory 1982, §110) and

$$D = YZ(y/Y), \tag{23}$$

where the function $Z(\cdot)$ is the Legendre dual of $X(x)$. This is still true even when $X = x$ so that $\partial Y/\partial x \equiv 0$, for then $D = 0$ and $Z(1) = 0$. The latter point is the pole of the polar $X = x$. The canonical transformation,

$$X = \tfrac{1}{3}x^3, \quad Y = yx^{-2}, \tag{24}$$

has the globally valid generating functions

$$A = \tfrac{1}{3}x^3Y, \quad C = -y(3X)^{\frac{1}{3}}, \quad D = \pm\tfrac{2}{3}Y(y/Y)^{\frac{3}{2}},$$

with $B = 0$ defined only on the curve $X = \tfrac{1}{3}x^3$.

In the next theorem we use suffixes to denote second derivatives of generating functions.

Theorem 7. *Whenever one or more of the four generating functions are available, we can express the first derivatives of a canonical transformation* (1) *in terms of the second derivatives of the generating functions as follows*:

$$\frac{\partial Y}{\partial y} = \frac{1}{A_{xY}} = -\frac{B_{XX}}{B_{Xx}} = -C_{Xy} + \frac{C_{XX}C_{yy}}{C_{Xy}} = -\frac{D_{yy}}{D_{Yy}}, \tag{25}$$

$$\frac{\partial X}{\partial y} = \frac{A_{YY}}{A_{xY}} = -\frac{1}{B_{Xx}} = -\frac{C_{yy}}{C_{Xy}} = -D_{Yy} + \frac{D_{YY}D_{yy}}{D_{Yy}}, \tag{26}$$

$$\frac{\partial X}{\partial x} = A_{xY} - \frac{A_{YY}A_{xx}}{A_{xY}} = -\frac{B_{xx}}{B_{Xx}} = -\frac{1}{C_{Xy}} = -\frac{D_{YY}}{D_{Yy}}, \tag{27}$$

$$\frac{\partial Y}{\partial x} = -\frac{A_{xx}}{A_{xY}} = B_{Xx} - \frac{B_{XX}B_{xx}}{B_{Xx}} = \frac{C_{XX}}{C_{Xy}} = -\frac{1}{D_{Yy}}. \tag{28}$$

A sufficient condition for the four A formulae to apply is that A_{xY} *be finite and non-zero; and similarly for* B_{Xx}, C_{Xy}, D_{Yy}.

Proof. Suppose $\partial Y/\partial y \neq 0, \pm\infty$, so that (10) and (14) apply, at least locally. Then

$$\partial A/\partial Y = X(x, Y), \quad \partial A/\partial x = y(x, Y). \tag{29}$$

Inserting the inverse $Y = Y(x, y)$ of $y = y(x, Y)$ into $(29)_2$, and differentiating with respect to y and x using the chain rule, gives

$$1 = A_{xY}\,\partial Y/\partial y, \quad 0 = A_{xx} + A_{xY}\,\partial Y/\partial x.$$

Inserting $Y = Y(x, y)$ into $(29)_1$ recovers the original $X = X(x, y)$, and differentiating that with respect to x and y using the chain rule gives

$$\frac{\partial X}{\partial x} = A_{xY} + A_{YY}\frac{\partial Y}{\partial x}, \quad \frac{\partial X}{\partial y} = A_{YY}\frac{\partial Y}{\partial y}.$$

The formulae stated in (25)–(28) in terms of $A(x, Y)$ emerge, under the single hypothesis that $A_{xY} \neq 0, \pm\infty$.

The other formulae in terms of B, C and D are obtainable by similar calculations. □

That a transformation (1) is canonical when the A formulae in (25)–(28) apply can be confirmed by direct calculation that $j = 1$, and likewise for the B, C and D formulae. We have not seen formulae (25)–(28) elsewhere.

5. More examples

(a) *Hodograph-related transformation*

When the cartesian components u, v of the plane velocity of a particle in a continuous medium are expressed as

$$u = u(x, y), \quad v = v(x, y) \tag{30}$$

in terms of functions on the right of the cartesian coordinates x, y of the current position of the particle, such a representation (30) is called the hodograph transformation from the physical space to the velocity space. The time is absence in steady flow, but it is present in unsteady flow, then acting as a parameter whose variation generates a sequence of hodograph transformations. The so-called hodograph method is a standard practical device in fluid mechanics (see Milne-Thomson, 1955, §20.3), and Whitney's theorem (1955) shows that the fold and cusp are the only stable singularities of (30) (cf. Sewell 1987, p. 158).

When the fluid is incompressible, (30) becomes (6). Comparison with (17), for example, and transcribing the neutral variables there to the physical ones here according to the scheme

$$\begin{array}{ccccc} D & Y & y & X & x \\ -\psi & x & y & v & u, \end{array}$$

shows that the stream function acts as a generating function leading to a canonical transformation

$$v = v(u, y), \quad x = x(u, y) \tag{31}$$

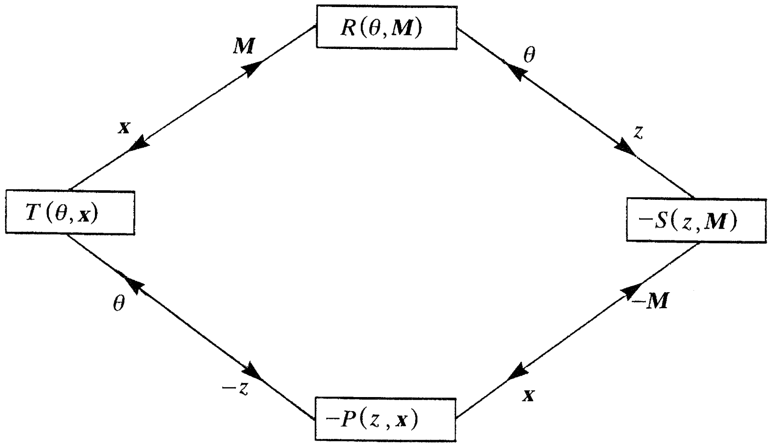

Figure 4. Legendre quartet in semi-geostrophic theory.

in terms of the fluid variables. This example is always available, except possibly near a point where $\partial^2\psi/\partial x\,\partial y = 0$ or $\pm\infty$, but even this might not be a global difficulty.

The particular stream function (7) generates, from (6), the velocity field

$$u = c - ca^2(x^2-y^2)/(x^2+y^2)^2, \quad v = -2ca^2xy/(x^2+y^2)^2 \tag{32}$$

with

$$\partial^2\psi/\partial x\,\partial y = -2ca^2x(x^2-3y^2)/(x^2+y^2)^3.$$

The singularity $D_{Yy} = 0$ thus occurs locally where $x = 0$, $\pm 3^{\frac{1}{2}}y$. Equation $(32)_1$ can be solved as

$$x^2 = -(y^2+\lambda) \pm (4\lambda y^2+\lambda^2)^{\frac{1}{2}} \quad \text{where} \quad 2\lambda = ca^2/(u-c)$$

to obtain $(31)_2$, and $(31)_1$ follows by substituting in $(32)_2$. This illustrates how a multivalued canonical transformation can result from a rather simple and single-valued generating function (7).

(b) *Semi-geostrophic theory*

The semi-geostrophic theory of meteorology provides a recent example of a generalization of figure 1, given by Chynoweth & Sewell (1989, 1991), which can contain singularities, and which is summarized in figure 4 in its own notation. Here $\boldsymbol{x}$ is a horizontal position vector in physical space, and the scalar z is a measure of height; $\boldsymbol{M}$ is a horizontal momentum vector, and θ is a measure of temperature. The transcriptions indicated by a direct comparison with figure 1 are

$$\begin{matrix} X & Y & x & y & A & B & C & D \\ \boldsymbol{M} & \boldsymbol{x} & \theta & -z & T & R & -S & -P. \end{matrix}$$

Each pair of arguments in figure 4 consists of a scalar with a vector, as distinct from the pairs of scalars in figure 1.

The scheme summarized by (20) again applies, but generalized to allow for the presence of vectors. For example, there is a Legendre transformation between

$R(\theta, \boldsymbol{M})$ and $P(z, \boldsymbol{x})$ at the top and bottom of figure 4, with all arguments active, having the properties

$$R+P = \boldsymbol{M}\cdot\boldsymbol{x}+\theta z,$$

$$\partial R/\partial\theta = z(\theta, \boldsymbol{M}), \quad \partial R/\partial \boldsymbol{M} = \boldsymbol{x}(\theta, \boldsymbol{M}), \tag{33}$$

$$\partial P/\partial z = \theta(z, \boldsymbol{x}), \quad \partial P/\partial \boldsymbol{x} = \boldsymbol{M}(z, \boldsymbol{x}) \tag{34}$$

(see Chynoweth *et al.* 1988; Purser & Cullen 1987).

The particular case of flow in a single vertical physical plane is commonly studied, and often with the objective of modelling the trace of an atmospheric front in that plane. The vectors $\boldsymbol{M}$ and $\boldsymbol{x}$ are now replaced by their scalar component values M and x. In general $(33)_1$ can now be inverted and substituted into $(33)_2$ to give a canonical transformation,

$$M = M(\theta, -z), \quad x = x(\theta, -z), \tag{35}$$

generated, for example, by $R(\theta, M)$.

A specific illustration is provided by the parabolic umbilic polynomial,

$$R(\theta, M) = \tfrac{1}{4}M^4 + M\theta^2 + \alpha M^2 + \beta\theta^2, \tag{36}$$

in which α and β are given parameters. This leads via (33) to

$$z = 2\theta(M+\beta), \quad x = M^3 + 2\alpha M + \theta^2,$$

which can be rearranged as the canonical transformation

$$M = z/2\theta - \beta, \quad x = (z/2\theta - \beta)^3 + 2\alpha(z/2\theta - \beta) + \theta^2. \tag{37}$$

The property

$$\partial(M, x)/\partial(\theta, -z) = 1 \tag{38}$$

can be immediately verified directly. The function (36) was used by Chynoweth *et al.* (1988) and Chynoweth & Sewell (1989) as a starting point for calculating its Legendre dual function $P(z, x)$, because the latter has a self-intersection line whose projection onto the physical x, z plane models the trace of an atmospheric front; across this there are jumps in the temperature and wind speed, which are represented by the gradients θ and M of $P(z, x)$ in (34). From the viewpoint of canonical transformations, (37) is therefore an example of one which is derivable from a multivalued generating function $P(z, x)$ possessing self-intersections. Convexification can then yield a single-valued version of $P(z, x)$ possessing a crease, representing the atmospheric front. This function, and the associated generating functions $T(\theta, x)$ and $S(z, M)$, are shown graphically by Chynoweth & Sewell (1989).

In a second and different illustration Chynoweth & Sewell (1989) emphasize the use of a variety of choices of $S(z, M)$ as a starting point for the construction of frontal models, because they also lead to self-intersections in $P(z, x)$. Canonical transformations (35) are generated by such $S(z, M)$ via

$$-\partial S/\partial z = \theta(z, M), \quad \partial S/\partial M = x(z, M) \tag{39}$$

followed by inversion, either of $(39)_1$ to substitute $M(\theta, -z)$ into $(39)_2$ to achieve (35), or of $(39)_2$ to substitute $z = z(M, x)$ into $(39)_1$ to achieve

$$\theta = \theta(M, x), \quad z = z(M, x). \tag{40}$$

The single-valued

$$S = \tfrac{1}{12}M^4 + \tfrac{1}{2}zM^2 \tag{41}$$

provides an illustration generating the canonical transformation

$$\theta = -\tfrac{1}{2}M^2, \quad -z = \tfrac{1}{3}M^2 - x/M, \tag{42}$$

which is an example of (22). It is easy to verify that

$$\partial(\theta, -z)/\partial(M, x) = 1.$$

The other three generating functions are shown in fig. 2 of Chynoweth & Sewell (1989) to be a swallowtail-shaped and therefore triple-valued $P(z, x)$, like figure 5 here, a double valued Cayley–Whitney umbrella $T(\theta, x) = \pm x(-2\theta)^{\frac{1}{2}} - \frac{1}{3}\theta^2$, and $R = \frac{1}{12}M^4$ defined only on the parabola $\theta = -\frac{1}{2}M^2$. Convexified and therefore single-valued versions of these can also be constructed.

(c) *Thermodynamics*

The four thermodynamic potential functions provide a classical example of figure 1. The Legendre transformations can contain isolated singularities, and the generating functions can be multivalued. This applies, in particular, to the van der Waals fluid, in which the Gibbs free enthalpy function $G(T, p)$ of temperature T and pressure p is swallowtail-shaped and therefore triple valued (see Sewell 1987, §2). The transcriptions between our neutral notation and a common thermodynamic notation are

X	Y	x	y	A	B	C	D
S	T	v	p	$-F$	U	$-H$	G,

where S is entropy, v is specific volume, F is free energy, U is internal energy and H is enthalpy. Therefore the relations

$$S = S(v, p), \quad T = T(v, p) \tag{43}$$

provide another example of a canonical transformation.

A simpler example than the van der Waals fluid is the ideal gas, for which

$$U(v, S) = c_v v^{1-\gamma} \exp((S-s)/c_v),$$

where γ, s and c_v are given constants. From its gradients (15)

$$T = v^{1-\gamma} \exp((S-s)/c_v), \quad p = (\gamma-1)\, c_v v^{-\gamma} \exp((S-s)/c_v).$$

Solving the second of these for S and substituting into the first gives the canonical transformation

$$S = s + c_v \ln pv^{\gamma}/(\gamma-1)\, c_v, \quad T = pv/(\gamma-1)\, c_v. \tag{44}$$

This time it is easily verified that

$$\partial(S, T)/\partial(v, p) = 1.$$

(d) *Numerical integration*

A comparison, given by Miller (1991), of two different numerical integration schemes indicates that the more reliable one is that which generates the solution via a sequence of canonical transformations (such a scheme is called a 'symplectic integrator'), in contrast to the one which does not preserve such a sequence. The former scheme is called a *time-centred leapfrog*

$$u^{(n+\frac{1}{2})} = u^{(n-\frac{1}{2})} + tf^{(n)}, \quad x^{(n+1)} = x^{(n)} + tu^{(n+\frac{1}{2})}. \tag{45}$$

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Here u denotes momentum per unit mass of a pendulum located at x, the force per unit mass is f which depends on x, and t is the integration time-step. Values at the old time-step are denoted by n, and those at the new one by $n+1$. The less reliable scheme is a predictor–corrector one.

The essence of the idea is to treat an iteration

$$x^{(n)} \rightarrow x^{(n+1)}, \quad u^{(n-\frac{1}{2})} \rightarrow u^{(n+\frac{1}{2})}, \tag{46}$$

with $f^{(n)}$ depending on $x^{(n)}$, as a transformation (1) via the transcriptions

$$\begin{array}{cccc} X & Y & x & y \\ x^{(n+1)} & u^{(n+\frac{1}{2})} & x^{(n)} & u^{(n-\frac{1}{2})}. \end{array}$$

Then writing $f^{(n)}(x^{(n)}) = F(x)$, (1) becomes

$$X = x + t^2 F(x) + ty, \quad Y = tF(x) + y. \tag{47}$$

It follows directly that $j = 1$, and since $t \neq 0$, that (10), (11), (14) and (15) always apply with

$$A(x, Y) = xY + \tfrac{1}{2}tY^2 - t\int^x F(\xi)\,\mathrm{d}\xi, \quad B(x, X) = \frac{1}{2t}(X-x)^2 + t\int^x F(\xi)\,\mathrm{d}\xi, \tag{48}$$

where ξ is a dummy integration variable.

To find the other two generating functions requires further information about $F(x)$. For example, $\mathrm{d}F/\mathrm{d}x \neq 0, \pm\infty$ is sufficient for a unique local inverse $F^{-1}(\cdot)$ (say) to exist such that

$$D(Y, y) = -\tfrac{1}{2}tY^2 - t\int^{(Y-y)/t} F^{-1}(\xi)\,\mathrm{d}\xi. \tag{49}$$

Again, writing $G(x) = x + t^2F(x)$, then $\mathrm{d}G/\mathrm{d}x \neq 0, \pm\infty$ is sufficient for a unique local inverse $G^{-1}(\cdot)$ (say) to exist such that

$$C(X, y) = -\frac{X^2}{2t} + \frac{1}{t}\int^{X-ty} G^{-1}(\xi)\,\mathrm{d}\xi. \tag{50}$$

6. Alternative definitions

Here we comment briefly on some of the other definitions of a canonical transformation which were referred to at the beginning of §2.

(a) *Existence of a generating function*

If a differentiable function $B(x, X)$ of independent variables x and X exists and is single valued, and if (15) holds, then its first differential is unambiguously

$$\mathrm{d}B = Y\,\mathrm{d}X - y\,\mathrm{d}x. \tag{51}$$

Carathéodory (1982, §86) begins with a definition that looks like this, i.e. that the transformation (1) is canonical if B exists such that (51) holds, except that his B is a function of x and y, not x and X. He moves quickly to a definition that, in the lowest dimensional case, is equivalent to our $j = 1$.

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We can see from Theorems 3 and 7 that it might seem reasonable to adopt a definition of the following type. 'The transformation (1) is canonical if at least one generating function exists, say $B(x,X)$, with properties represented by (15) with $B_{xX} \neq 0, \pm\infty$.' However, this uses the benefit of hindsight, it is unsymmetrical in requiring four options to be checked out, and it entails more assumptions about the differentiability of (1) than does the very direct definition that $j = 1$. So such a definition implies $j = 1$, but is not implied by it, and therefore the two are not equivalent.

Moreover, we have deduced that generating functions can be multivalued, can possess self-intersections, and can be restricted to domains of less than the fully permitted dimension. It would be difficult to describe these global and local specifications in advance.

The following question is a prototype of one which arises in the study of contact transformations (Carathéodory 1982, §120). What transformations of type (1) can have the property

$$Y\,\mathrm{d}X = y\,\mathrm{d}x \tag{52}$$

of local invariance of this particular differential form, and can they be described as canonical in some sense? From the discussion after Theorem 6 we can see that any transformation of the form

$$X = X(x), \quad Y = y/(\mathrm{d}X/\mathrm{d}x) \tag{53}$$

with $\mathrm{d}X/\mathrm{d}x \neq 0, \ \pm\infty$ satisfies (52) and has $j = 1$. The associated generating functions are

$$A(x,Y) = YX(x), \quad C(X,y) = -yx(X), \quad D(Y,y) = YZ(y/Y), \tag{54}$$

with $B(x,X) \equiv 0$ defined only on the curve $X = X(x)$. The inverse and the Legendre dual of $X(x)$ are $x(X)$ and $Z(\cdot)$ respectively. Thus (52) implies $j = 1$, and also that $B(x,X)$ is defined only on a restricted domain and has the value zero there.

(b) *Invariance of a circuit integral*

If $B(x,X)$ has a single-valued branch over a closed curve drawn in its domain, then it follows from (51) that

$$\oint Y\,\mathrm{d}X = \oint y\,\mathrm{d}x, \tag{55}$$

where the circuit integrals are each evaluated around the lifted version of the curve drawn on the considered branch.

This result expresses the invariance of the circuit integral under the transformation (1) which is obtained by inverting $y = y(x,X)$ given by $(15)_1$ as $(1)_1$ and inserting into $(15)_2$.

Similar hypotheses on $A(x,Y)$, $C(X,y)$ or $D(Y,y)$ lead to similar invariance properties

$$\oint X\,\mathrm{d}Y = -\oint y\,\mathrm{d}x, \quad \oint Y\,\mathrm{d}X = -\oint x\,\mathrm{d}y, \quad \oint X\,\mathrm{d}Y = \oint x\,\mathrm{d}y, \tag{56}$$

respectively.

Another possible definition is the following. 'The transformation (1) is canonical if at least one of the invariance properties in (55) and (56) holds.' According to Arnold (1989, §§44E and 45A), a definition of this type is the generally accepted one, and implies others which he quotes (cf. Schutz 1980). Even if it is taken to imply the

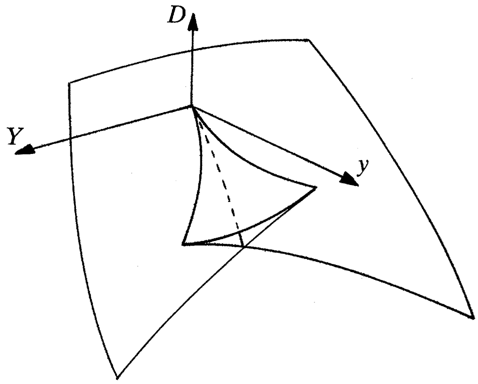

Figure 5. Swallowtail $D(Y, y)$.

existence of a single-valued generating function, when reference to the lifted version of the circuit becomes redundant, it is not equivalent to the other definitions reviewed here, and it is subject to the following qualifications.

We have given specific examples in §§5*b*, *c* in which $D(Y, y)$ has the swallowtail shape of the general type represented in figure 5. It must be a reasonable expectation that a generating function has global multivaluedness, e.g. of the type shown in figure 3 or figure 5, or worse in higher dimensions.

In such circumstances, if one seeks to use invariance of a circuit integral such as $(56)_3$ as the defining property of a canonical transformation, one must decide which single-valued part of the multivalued generating function is to receive the lifted circuit. It may be that at least one of the four generating functions is always globally single valued, but in the absence of a theorem which identifies which one, there is an inherent ambiguity in the use of circuit integral invariance as the definition of a canonical transformation. Definitions phrased in terms of manifolds, which are single valued *ipso facto*, may offer only formal understanding.

(*c*) *Invariance of the Poisson bracket*

Let $F(X, Y)$ and $G(X, Y)$ be any two differentiable functions of X and Y. Their Poisson bracket is defined to be

$$[F, G] = \frac{\partial F}{\partial X}\frac{\partial G}{\partial Y} - \frac{\partial F}{\partial Y}\frac{\partial G}{\partial X}.$$

Suppose the transformation (1), whether canonical or not, converts F and G into two new functions

$$f(x, y) = F(X, Y) \quad \text{and} \quad g(x, y) = G(X, Y) \tag{57}$$

without changing their values. The Poisson bracket of the new functions is

$$[f, g] = \frac{\partial f}{\partial x}\frac{\partial g}{\partial y} - \frac{\partial f}{\partial y}\frac{\partial g}{\partial x}.$$

Theorem 8. *A canonical transformation* (1) *with* (2) *will leave the value of the Poisson bracket invariant, i.e.*

$$[F, G] = [f, g], \tag{58}$$

when the sufficient hypotheses of Theorem 2 hold.

If (58) *holds for a transformation* (1) *which is not required to satisfy* (2) *a priori, then either* $j=1$ *or*

$$\frac{\partial F}{\partial X}\frac{\partial g}{\partial y}-\frac{\partial f}{\partial y}\frac{\partial G}{\partial X}=0, \tag{59}$$

under the same sufficient hypotheses.

Proof. Suppose that $\partial Y/\partial y \neq 0, \pm\infty$ in $(1)_2$ so that, at least locally, there is a single-valued inverse $y=y(x,Y)$ which can be used in $(1)_2$ to give $X=X(x,Y)$. Then (57) can also be expressed as new functions $\bar{f}(x,Y)$ and $\bar{g}(x,Y)$ say, respectively, in terms of x and Y as independent variables. The chain rule then gives

$$\frac{\partial \bar{f}}{\partial Y}=\frac{\partial f}{\partial y}\frac{\partial y}{\partial Y}=\frac{\partial F}{\partial Y}+\frac{\partial F}{\partial X}\frac{\partial X}{\partial Y}, \quad \frac{\partial \bar{g}}{\partial x}=\frac{\partial g}{\partial y}\frac{\partial y}{\partial x}=\frac{\partial G}{\partial X}\frac{\partial X}{\partial x}$$

in terms of the derivatives of $y(x,Y)$ and of $X(x,Y)$. Hence

$$\frac{\partial f}{\partial y}\left(\frac{\partial g}{\partial x}+\frac{\partial g}{\partial y}\frac{\partial y}{\partial x}\right)=\frac{\partial f}{\partial y}\frac{\partial G}{\partial X}\frac{\partial X}{\partial x}, \quad \frac{\partial G}{\partial X}\left(\frac{\partial F}{\partial Y}+\frac{\partial F}{\partial X}\frac{\partial X}{\partial Y}\right)=\frac{\partial G}{\partial X}\frac{\partial f}{\partial y}\frac{\partial y}{\partial Y}.$$

Similarly, by interchanging the roles of f and g, and of F and G,

$$\frac{\partial g}{\partial y}\left(\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}\frac{\partial y}{\partial x}\right)=\frac{\partial g}{\partial y}\frac{\partial F}{\partial X}\frac{\partial X}{\partial x}, \quad \frac{\partial F}{\partial X}\left(\frac{\partial G}{\partial Y}+\frac{\partial G}{\partial X}\frac{\partial X}{\partial Y}\right)=\frac{\partial F}{\partial X}\frac{\partial g}{\partial y}\frac{\partial y}{\partial Y}.$$

Subtracting this latter pair of equations from the previous pair gives

$$[f,g]=\left(\frac{\partial F}{\partial X}\frac{\partial g}{\partial y}-\frac{\partial f}{\partial y}\frac{\partial G}{\partial X}\right)\frac{\partial X}{\partial x}, \quad [F,G]=\left(\frac{\partial F}{\partial X}\frac{\partial g}{\partial y}-\frac{\partial f}{\partial y}\frac{\partial G}{\partial X}\right)\frac{\partial y}{\partial Y}.$$

Hence, after using a result derived during the proof of Theorem 2,

$$[f,g]-[F,G]=\left(\frac{\partial F}{\partial X}\frac{\partial g}{\partial y}-\frac{\partial f}{\partial y}\frac{\partial G}{\partial X}\right)\frac{\partial y}{\partial Y}(j-1) \tag{60}$$

without yet assuming that the transformation (1) is canonical, and in which $\partial y/\partial Y \neq 0, \pm\infty$. Similar formulae will follow from the other three hypotheses in Theorem 2.

Now using $j=1$ for the first time in the proof delivers (58). Conversely, if (58) is assumed without (2), then we deduce from (60) or one of the three similar formulae that either $j=1$ or (59) holds. □

Occasionally the following definition is adopted, without requiring $j=1$, for example by Sudarshan & Mukunda (1974) and Woodhouse (1987). 'The transformation (1) is canonical if (58) applies for every pair of functions (57).' This is designed to exclude the possibility of (59). The purpose of Theorem 8 is to clarify comparison with our definition which just requires $j=1$. The formula (60) will help the reader to make his or her own judgement about the choice of definition.

(d) *Invariance of hamiltonian structure*

Some authors, including Synge (1960, §87), start with the following definition: 'The transformation (1) is canonical if it leaves invariant both the form of Hamilton's equations (5) and the value of the hamiltonian function'. We have already indicated this, in §§1 and 3.

(*e*) *Contact geometry*

Whittaker (1937) does not use the term 'canonical transformation'. Instead (p. 290) he uses 'contact transformation' following Lie, in the context of wave fronts in particular, and he applies this name to our example (3) of a canonical transformation. Goldstein (1950, p. 239) treats the two terms as synonymous. Plainly they are not so, however, if a contact transformation is defined in terms of reciprocation. For a Legendre transformation can be defined as a mapping between the envelope of a polar plane and the locus of a pole. In that sense it is a contact transformation, but it is certainly not a canonical transformation in the sense of $j = 1$. Also, a Legendre transformation can be a mapping between sets of odd numbers of variables just as easily as even numbers (e.g. pairs). We have not needed otherwise to invoke ideas of contact geometry, except for the remark at the end of §6*a*, and we defer further comment on that large subject.

7. Higher dimensions

The main purpose of this paper has been to learn from the explicit precision and examples which can be displayed for canonical transformations of the plane onto the plane. We shall not pursue here the arguments of very different styles which are required in higher dimensions, such as are found in Carathéodory (1982), Synge (1960) and Arnold (1989), for example. Instead we conclude with a higher dimensional version of Theorem 7, which we have not seen elsewhere.

Suppose that a pair of n-tuples $x_1, \ldots, x_n$ and $y_1, \ldots, y_n$ of real scalars is related to another such pair $X_1, \ldots, X_n$ and $Y_1, \ldots, Y_n$ by

$$X_i = X_i(x_j, y_j), \quad Y_i = Y_i(x_j, y_j). \tag{61}$$

An isolated suffix takes each of its values in turn, so that the expressions on the right represent $2n$ differentiable functions, each of $2n$ variables, and the same symbol is used for a function and its values. Thus (61) generalizes (1).

Theorem 9. *Suppose that the determinant*

$$|\partial Y_i/\partial y_j| \neq 0, \pm\infty. \tag{62}$$

Suppose also that a twice differentiable scalar generating function $A(x_j, Y_j)$ exists such that

$$\partial A/\partial Y_i = X_i(x_j, Y_j), \quad \partial A/\partial x_i = y_i(x_j, Y_j). \tag{63}$$

Then the first derivatives of (61) *can be expressed in terms of the second derivatives of $A(x_j, Y_j)$ by the following formulae.*

$$\partial Y_k/\partial y_j = A^{-1}_{x_j Y_k}, \quad \partial Y_k/\partial x_j = -A^{-1}_{x_l Y_k} A_{x_l x_j}, \tag{64}$$

$$\partial X_i/\partial x_j = A_{Y_i x_j} - A_{Y_i Y_k} A^{-1}_{x_l Y_k} A_{x_l x_j}, \quad \partial X_i/\partial y_j = A_{Y_i Y_k} A^{-1}_{x_j Y_k}. \tag{65}$$

The inverse notation is explained in the proof. Summation is implied by a repeated suffix.

Proof. Condition (62) is sufficient for the inverse $y_i = y_i(x_j, Y_j)$ of $(61)_2$ to be uniquely available locally. This inverse is on the right of $(63)_1$. Therefore inserting $(61)_2$ into $(63)_2$ and differentiating with respect to y_j and x_j, using the chain rule, gives

$$\delta_{ij} = A_{x_i Y_k} \partial Y_k/\partial y_j, \quad 0 = A_{x_i x_j} + A_{x_i Y_k} \partial Y_k/\partial x_j. \tag{66}$$

Inserting $(61)_2$ into $(63)_1$ recovers the original $(61)_1$, so differentiating $(63)_1$ with respect to x_j and y_j, using the chain rule, gives

$$\frac{\partial X_i}{\partial x_j} = A_{Y_i x_j} + A_{Y_i Y_k}\frac{\partial Y_k}{\partial x_j}, \quad \frac{\partial X_i}{\partial y_i} = A_{Y_i Y_k}\frac{\partial Y_k}{\partial y_j}. \tag{67}$$

To solve these, we first notice by taking the determinants of $(66)_1$ that (62) is equivalent to

$$|A_{x_i Y_k}| \neq 0, \pm\infty. \tag{68}$$

Hence the symmetric $n \times n$ matrix with typical component $A_{x_i Y_k} = \partial^2 A/\partial x_i \, \partial Y_k$ is non-singular, and therefore has an inverse, whose typical component we denote by $A^{-1}_{x_i Y_k}$ (this is not the reciprocal of the typical component $A_{x_i Y_k}$ itself). Hence

$$A^{-1}_{x_i Y_j} A_{x_i Y_k} = \delta_{jk}. \tag{69}$$

Therefore (66) gives (64), so that (67) gives (65). □

The jacobian of (61) can be denoted by

$$j = \partial(X_i, Y_i)/\partial(x_i, y_i).$$

By the chain rule for jacobians, under hypothesis (62),

$$j = \frac{\partial(X_i, Y_i)}{\partial(x_i, Y_i)}\frac{\partial(x_i, Y_i)}{\partial(x_i, y_i)} = \frac{\partial(X_i)}{\partial(x_i)}\frac{\partial(Y_i)}{\partial(y_i)}$$

in the alternative notation for jacobians. Therefore the jacobians of the right sides of (63) satisfy

$$\frac{\partial(X_i)}{\partial(x_i)} = j\frac{\partial(y_i)}{\partial(Y_i)}. \tag{70}$$

Therefore, if (61) is canonical in the sense that $j = 1$, (70) becomes

$$\frac{\partial(X_i)}{\partial(x_i)} = \frac{\partial(y_i)}{\partial(Y_i)}, \tag{71}$$

which is an integrability condition necessary but not (unless $n = 1$) sufficient for the existence of $A(x_j, Y_j)$ hypothesized in (63).

Sufficient integrability conditions when $n > 1$ are conveniently expressed by changing the notation to the sets

$$\{Z_\alpha\} = \{X_i, Y_i\}, \quad \{z_\beta\} = \{x_i, y_i\} \quad \text{for} \quad \alpha, \beta = 1, \ldots, 2n.$$

Then if the $2n$ functions $Z_\alpha(z_\beta)$ each of $2n$ variables satisfy

$$\partial Z_\alpha/\partial z_\beta = \partial Z_\beta/\partial z_\alpha \quad \text{for all} \quad \alpha, \beta, \tag{72}$$

there exists a scalar function $F(z_\alpha)$ such that

$$Z_\alpha = \partial F/\partial z_\alpha. \tag{73}$$

Necessity of (72) (and hence (71)) is obvious. Sufficiency is based on choosing a datum point $\{a_\alpha\}$ and constructing the function

$$F(z_1, \ldots, z_{2n}) = \sum_{\alpha=1}^{2n} \int_{a_\alpha}^{z_\alpha} Z_\alpha(z_1, \ldots, z_{\alpha-1}, t, a_{\alpha+1}, \ldots, a_{2n}) \, dt. \tag{74}$$

By using (72) we see that this has the gradients

$$\begin{aligned}\frac{\partial F}{\partial z_\beta} &= Z_\beta(z_1,\dots,z_\beta,a_{\beta+1},\dots,a_{2n})\\ &\quad+\sum_{\alpha>\beta}\int_{a_\alpha}^{z_\alpha}\frac{\partial Z_\alpha}{\partial z_\beta}(z_1,\dots,z_{\alpha-1},t,a_{\alpha+1},\dots,a_{2n})\,\mathrm{d}t\\ &= Z_\beta(z_1,\dots,z_\beta,a_{\beta+1},\dots,a_{2n})\\ &\quad+\sum_{\alpha>\beta}\int_{a_\alpha}^{z_\alpha}\frac{\partial Z_\beta}{\partial z_\alpha}(z_1,\dots,z_{\alpha-1},t,a_{\alpha+1},\dots,a_{2n})\,\mathrm{d}t\\ &= Z_\beta(z_1,\dots,z_\beta,a_{\beta+1},\dots,a_{2n})\\ &\quad+\sum_{\alpha>\beta}[Z_\beta(z_1,\dots,z_\alpha,a_{\alpha+1},\dots,a_{2n})-Z_\beta(z_1,\dots,z_{\alpha-1},a_\alpha,\dots,a_{2n})]\\ &= Z_\beta(z_1,\dots,z_{2n}).\end{aligned}$$

We thank Dr D. S. G. Stirling for drawing our attention to this construction. Quite different looking versions of an associated result are known as Frobenius's theorem (see Schutz 1980; Flanders 1963).

8. Conclusions

In this paper we have given some new examples of canonical transformations. We have shown that the generating functions of such transformations can be globally multivalued, like the swallowtail, in some cases, and that the dimension of their domain of definition can be restricted, in other cases. Some of these examples spring from a meteorological context, in the analysis of atmospheric fronts. Another reason for interest in canonical (sometimes called symplectic) transformations stems from their role in symplectic integrators. These are numerical algorithms, based on generating functions, for the solution of equations of hamiltonian type, which preserve the hamiltonian structure during the approximation.

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