Equivalence to Thermodynamic Functions Induced in Nonlinear Systems by Symmetries of Transformation Groups

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Characteristic functions have been defined in nonlinear autonomous systems. These functions possess properties which are equivalent to those of the energy and the entropy concepts of thermodynamics. The new functions are induced in nonlinear systems by one parameter transformation groups. The mathematical treatment is based on canonical forms and their transformation.

In recent years, the thermodynamic aspect [1] common to chemical reaction systems and electronic ones has been emphasized. Both kinds of system are treated in the theory of thermodynamics of irreversible processes. Hence, all thermodynamic properties known from chemical systems should also apply to their electronic equivalents and general characteristic features of electronic systems should have a counter part in chemical systems. Thus, it has been shown that chemical reaction schemes represent a structure similar to that of the electronic network which is well known from circuit diagrams. A knowledge of the network (e.g. the circuit diagram or the reaction scheme) in both cases permits the construction of a set of differential equations, which describes the dynamics of the system. The differential equations have the general form:

$$\frac{d}{dt} x_i = f_i(x_j), \quad (i, j = 1, 2, \ldots, n)$$

where the left hand side represents the time derivative of quantities x_i (e.g. concentrations or electrical charges) and the right hand side displays functions f_i of quantities only. Note, that the functions are time independent (i.e. the system is autonomous). The special structure of the system and the characteristics of its constitutive components is coded in the functions f_i.

So far, the system seems to be completely described by the set of differential equations, hence capable of delivering all its properties. However, the thermodynamic aspect of the system demands that the laws of energy and entropy also are valid for such systems, but examination of the differential equations does not easily reveal how such functions could be evaluated. Moreover, the physical chemistry teaches that also several other potential energy functions (e.g. enthalpy, Gibbs-energy, etc.) exist.

In this paper, we analyse the relations of one-parameter groups to differential forms inherent in autonomous differential systems. The potential functions in thermodynamics are expressed in differential forms. Our main objective is to construct a function for autonomous systems (e.g. as electronic ones) which corresponds to entropy, for chemical reactions. This must be possible since the essential features characterizing any thermodynamic system are inherent in the entropy. Entropy can only be produced and is closely related to the structural order of the system. Since systems with only two variables x_i ($i = 1, 2$) cannot demonstrate the phenomena clearly, we have extended the chemical model of Dreitlein and Smoes (a system of two variables) to three variables. We shall analyse this model with respect to the one-parameter groups it admits and try to interpret the functions obtained by subjecting the model to transformations which carry it into a canonical form. This article is an extension of a previous contribution [2] and contains many ideas developed in that paper. Thus, readers who are not familiar with the use of one-parameter groups in systems theory are recommended to consult the preceding work.

Transformation of a System into a Canonical Form

Since already a system with only three variables displays the properties to be discussed, we shall

restrict ourselves to treat such systems. Subsequently, it is easy to generalize the formalisms to higher numbers of variables.

An autonomous system in three variables:

$$\dot{x}_1 = f_1(x_1, x_2, x_3),$$
$$\dot{x}_2 = f_2(x_1, x_2, x_3), \qquad (1\,a)$$
$$\dot{x}_3 = f_3(x_1, x_2, x_3)$$

is, according to the one-parameter theory of groups, associated with a vector field [3], (infinitesimal generator) A':

$$A' = f_1 \frac{\partial}{\partial x_1} + f_2 \frac{\partial}{\partial x_2} + f_3 \frac{\partial}{\partial x_3}. \qquad (1\,b)$$

The canonical form theorem [4] of one-parameter groups states that by a proper change of the coordinates of the variables (i.e. $(x_1, x_2, x_3) \rightarrow (x_1{}^*, x_2{}^*, x_3{}^*)$), the generator A' can be transformed into another generator A^* (see Eq. (24) of paper [5])

$$A^* = A'x_1{}^* \frac{\partial}{\partial x_1{}^*} + A'x_2{}^* \frac{\partial}{\partial x_2{}^*} \qquad (A)$$
$$+ A'x_3{}^* \frac{\partial}{\partial x_3{}^*}.$$

If $A'x_2{}^* = A'x_3{}^* = 0$; $A'x_1{}^* = 1$ are chosen, it takes the simple form:

$$A^* = \partial/\partial x_1{}^*.$$

Another generator U' will be transformed by the same transformation into:

$$U^* = U'x_1{}^* \frac{\partial}{\partial x_1{}^*} + U'x_2{}^* \frac{\partial}{\partial x_2{}^*}$$
$$+ U'x_3{}^* \frac{\partial}{\partial x_3{}^*}.$$

A second change of the coordinates i.e. $(x_1{}^*, x_2{}^*, x_3{}^*) \rightarrow (x_1{}^{**}, x_2{}^{**}, x_3{}^{**})$ carries A^* into A^{**} and U^* into

$$U^{**} = U^* x_1{}^{**} \frac{\partial}{\partial x_1{}^{**}} + U^* x_2{}^{**} \frac{\partial}{\partial x_2{}^{**}}$$
$$+ U^* x_3{}^{**} \frac{\partial}{\partial x_3{}^{**}}.$$

If the new coefficients of the partial derivatives are chosen:

$$A^* x_1{}^{**} = 1, \quad A^* x_2{}^{**} = A^* x_3{}^{**} = 0, \qquad (a)$$
$$U^* x_1{}^{**} = ?, \quad U^* x_2{}^{**} = 1, \quad U^* x_3{}^{**} = 0 \quad (b)$$

a simplified form is obtained where Eqs. (a) imply that $x_2{}^{**}$ and $x_3{}^{**}$ are independent of $x_1{}^*$ and that $x_1{}^{**} = x_1{}^* + f(x_2{}^*, x_3{}^*)$. Now, the last two Eqs. (b)

$$u_2{}^* \frac{\partial x_2{}^{**}}{\partial x_2{}^*} + u_3{}^* \frac{\partial x_2{}^{**}}{\partial x_3{}^*} = 1;$$
$$u_2{}^* \frac{\partial x_2{}^{**}}{\partial x_2{}^*} + u_3{}^* \frac{\partial x_3{}^{**}}{\partial x_3{}^*} = 0$$

may be solved for $x_2{}^{**}$ and $x_3{}^{**}$, so that the simpler form (b) is valid. In general, it will not be possible by this technique to reduce the first Eq. (b) into a simple expression, since the differential equation $U^*x_1{}^{**}$ contains $x_1{}^*$, whereas the arbitrary function f, which is available to reduce the equation only is dependent upon the variables $x_2{}^*$ and $x_3{}^*$. Hence, by this second transformation the two generators A' and U' take the form:

$$A^{**} = \frac{\partial}{\partial x_1{}^{**}},$$
$$U^{**} = g_1{}^*(x_1{}^{**}, x_2{}^{**}, x_3{}^{**}) \frac{\partial}{\partial x_1{}^{**}} + \frac{\partial}{\partial x_2{}^{**}}.$$

The same procedure may be applied to an additional generator U_2' to give the generator system:

$$A^{***} = \frac{\partial}{\partial u},$$
$$U_1{}^{***} = g_1(u, v, w) \frac{\partial}{\partial u} + \frac{\partial}{\partial v}, \qquad (2)$$
$$U_2{}^{***} = g_2(u, v, w) \frac{\partial}{\partial u} + k_2(u, v, w) \frac{\partial}{\partial v} + \frac{\partial}{\partial w},$$

where u, v, w are the new variables.

Hence, the general law of a canonical form says that an aggregate of infinitesimal generators can be transformed into a triangular form, in which the diagonal coefficients are 1.

One-parameter Groups and Common Solutions

The Eqs. (2) may be further reduced by use of their common solutions. Therefore, Eqs. (2) are rewritten by omitting the *** superscript and replacing terms on the right hand side by those of the left hand side, whenever possible:

$$A = \partial/\partial u,$$
$$U_1 = g_1 A + \partial/\partial v, \qquad (3)$$
$$U_2 = (g_2 - k_2 g_1) A + k_2 U_1 + \partial/\partial w.$$

Moreover, in the same way their commutators may be evaluated to:

$$[A, U_1] = (A\,g_1)\,A\,,$$
$$[A, U_2] = \{A\,(g_2 - k_2\,g_1)\}\,A + (A\,k_2)\,U_1, \quad (4)$$
$$[U_1, U_2] = \{U_1 g_2 - g_1 U_1 k_2 - U_2 g_1\}\,A$$
$$\qquad\qquad + (U_1 k_2)\,U_1\,.$$

The complete systems theorem [4] states that if a function $\Phi(u, v, w)$ is a common solution of two generators, e.g. A and U_1, then it is also a solution of its commutator, here $[A, U_1]$, and then the commutator may be represented by a linear combination of the generators, i.e.:

$$[A, U_1] = a_1\,A + a_2\,U_1$$

where a_1, a_2 are coefficients.

From Eqs. (4), one derives: the generators A and U_1 form a complete system with a common solution, but the generator pairs A, U_2 and U_1, U_2 do not in general form a complete system. The pair A, U_2 form a complete system if $A\,k_2 = 0$, i.e. if k_2 is a solution of the generator A. Moreover, from the condition $A\,k_2 = 0$ follows that, U_1 and U_2 are generators of groups admitted by the generator A, since they valididate the condition $[A, U_i] = \lambda_i A$ where λ is an arbitrary function. The groups U_1 and U_2 then transform solutions of A into their like.

Another important result is obtained from the common solution Φ of all the three generators A, U_1, U_2. Since with $A\Phi = U_1\Phi = U_2\Phi = 0$, a linear equation system exists, which only admits solutions other than constants if the determinant is zero. Since the determinant of Eqs. (3) is one, the system has no other common solutions than trivial ones.

The common solution of A and U_1 is $\Phi_1(w)$. For A and U_2, one obtains the simple common solution $\Phi_2(v)$ if $k_2 = 0$. Hence, the common solutions of A and the groups it admits are the independent solutions v and w of A. The general solution of A is an arbitrary function of v and w, $F(v, w)$. If k_2 is a solution of A, then the common solution of A and U_2 (see Eqs. (3)) satisfies

$$k_2\,\frac{\partial\Phi}{\partial v} + \frac{\partial\Phi}{\partial w} = 0 \quad \text{where} \quad k_2 = k_2(v, w)\,.$$

In case $k_2 \neq 0$, Φ will be a more complex function as for $k_2 = 0$. Thus the incorporation of solutions k_2 of A into the generators which it admits, changes the simple form of the common solution into a more complex one. But Φ will remain an independent solution of A.

An essential feature is revealed by supplementing the generator system with the total differential of the common function, e.g.

$$0 = A\,\Phi = \frac{\partial\Phi}{\partial u}\,,$$
$$0 = U_1\Phi = g_1\frac{\partial\Phi}{\partial u} + \frac{\partial\Phi}{\partial v}\,,$$
$$0 = \mathrm{d}\Phi = \mathrm{d}u\,\frac{\partial\Phi}{\partial u} + \mathrm{d}v\,\frac{\partial\Phi}{\partial v} + \mathrm{d}w\,\frac{\partial\Phi}{\partial w}\,.$$

The linear equation system in the derivatives only has a non-trivial solution if the determinant of its coefficient is zero; i.e. $\mathrm{d}w = 0$. The resulting differential form gives on integration the common solution. Since U_1 and U_2 in general have no common solution, they are associated with a non-integrable differential form μ, that is derived from

$$\mathrm{d}\Phi = \mathrm{d}u\,\frac{\partial\Phi}{\partial u} + \mathrm{d}v\,\frac{\partial\Phi}{\partial v} + \mathrm{d}w\,\frac{\partial\Phi}{\partial w}\,,$$
$$U_1\Phi = g_1\frac{\partial\Phi}{\partial u} + \frac{\partial\Phi}{\partial v}\,,$$
$$U_2\Phi = g_2\frac{\partial\Phi}{\partial u} + k_2\frac{\partial\Phi}{\partial v} + \frac{\partial\Phi}{\partial w}$$

as

$$\mu = \mathrm{d}u - g_1\,\mathrm{d}v - (g_2 - g_1\,k_2)\,\mathrm{d}w\,. \quad (5)$$

In summary, the consideration of the common solutions has yielded two results: Firstly, the differential form Eq. (5) that is inherent in the total of groups admitted by the differential equation system Eq. (1) and secondly that there is no common solution to the Eqs. (3) since the determinant of coefficients is one. Next, we shall investigate these properties under a change of variables.

Change of Variables

In the section ahead it is shown that, an autonomous system can be transformed into a canonical one. Now, we proceed the other way around. Starting with a canonical system we derive by successive transformation other more complex systems. The model of a chemical system, proposed by Dreitlein and Smoes [5] has previously [6] been treated in detail and also shall serve here for demonstration. This model, which only has two variables, has to be extended to a model with three variables (i.e. a

spherical model) to cover the aspect to be displayed. As previously, the transformation to new variables is performed in steps. In the first step, the new variables (r, φ, ϑ) are introduced instead of (u, v, w). After the transformation, the differential equations of the model:

$$\frac{dr}{dt} = \frac{\partial r}{\partial u}\frac{du}{dt} + \frac{\partial r}{\partial v}\frac{dv}{dt} + \frac{\partial r}{\partial w}\frac{dw}{dt} = r(r^2 - E),$$

$$\frac{d\varphi}{dt} = \frac{\partial \varphi}{\partial u}\frac{du}{dt} + \frac{\partial \varphi}{\partial v}\frac{dv}{dt} + \frac{\partial \varphi}{\partial w}\frac{dw}{dt} = -K, \quad (6)$$

$$\frac{d\vartheta}{dt} = \frac{\partial \vartheta}{\partial u}\frac{du}{dt} + \frac{\partial \vartheta}{\partial v}\frac{dv}{dt} + \frac{\partial \vartheta}{\partial w}\frac{dw}{dt} = -S$$

display a multiplicity, since $dv/dt = dw/dt = 0$, i.e. the determinant of the coefficients is always zero. This implies that several transformations (r, φ, ϑ) represent the same resulting model system which is given by the right hand side of (6). Inserting $dv = dw = 0$ and $du/dt = 1$ into (6), a set of equations is obtained:

$$\frac{\partial r}{\partial u} = r(r^2 - E), \frac{\partial \varphi}{\partial u} = -K, \frac{\partial \vartheta}{\partial u} = -S \quad (7)$$

which after replacement of u by t is equivalent to the set of the model system. The transformations

are obtained from the solution of Eqs. (7) by assuming that the integration constants c_1, c_2 and c_3 are functions of the cyclic variables v and w. All transformations:

$$r^2 = \frac{E}{1 - \exp[2E \cdot (u + c_1(v, w)]}$$
$$\varphi = -K(u - c_2(v, w)), \quad (8)$$
$$\vartheta = -S(u - c_3(v, w))$$

will result in the same Eqs. (6) of the model system.

The change of variables (Eqs. (8)) will according to the rule (A) transform the set of canonical generators Eqs. (3):

$$A^* = r(r^2 - E)\frac{\partial}{\partial v} - K\frac{\partial}{\partial \varphi} - S\frac{\vartheta}{\partial \vartheta},$$

$$U_1{}^* = g_1 A^* + \left\{ r(r^2 - E)\cdot\frac{\partial c_1}{\partial v}\frac{\partial}{\partial v} \right. \quad (9)$$

$$\left. - K\frac{\partial c_2}{\partial v}\frac{\partial}{\partial \varphi} - S\frac{\partial c_3}{\partial v}\frac{\partial}{\partial \vartheta} \right\},$$

$$U_2{}^* = (g_2 - k_2 g_1) A^* + k_2 U_1{}^*$$

$$+ r(r^2 - E)\frac{\partial c_1}{\partial w}\frac{\partial}{\partial v} - K\frac{\partial c_2}{\partial w}\frac{\partial}{\partial \varphi} - S\frac{\partial c_3}{\partial w}\frac{\partial}{\partial \vartheta}.$$

In matrix notation, these generators may be factorized:

$$\begin{pmatrix} A^* \\ U_1{}^* \\ U_2{}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ g_1 & 1 & 0 \\ g_2 & k_2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ \dfrac{\partial c_1}{\partial v} & \dfrac{\partial c_2}{\partial v} & \dfrac{\partial c_3}{\partial v} \\ \dfrac{\partial c_1}{\partial w} & \dfrac{\partial c_2}{\partial w} & \dfrac{\partial c_3}{\partial w} \end{pmatrix} \begin{pmatrix} r(r^2 - E) & 0 & 0 \\ 0 & -K & 0 \\ 0 & 0 & -S \end{pmatrix} \begin{pmatrix} \dfrac{\partial}{\partial v} \\ \dfrac{\partial}{\partial \varphi} \\ \dfrac{\partial}{\partial \vartheta} \end{pmatrix}. \quad (10)$$

The new generators have a common solution, if the determinants of the matrices are zero:

$$K S r(r^2 - E) \cdot \begin{vmatrix} 1 & 1 & 1 \\ \dfrac{\partial c_1}{\partial v} & \dfrac{\partial c_2}{\partial v} & \dfrac{\partial c_3}{\partial v} \\ \dfrac{\partial c_1}{\partial w} & \dfrac{\partial c_2}{\partial w} & \dfrac{\partial c_3}{\partial w} \end{vmatrix} = 0. \quad (11)$$

The conditions for the existence of a common solution contain factors which are independent of the arbitrary functions c_1, c_2, c_3 and a factor, that solely is dependent upon these functions. The Eqs. (11) represent a surface in space of the new variables (r, φ, ϑ) and is closely related to the singularities of the Equations (6).

In general, the change of variables from a triple (u, v, w) to a triple (u^*, v^*, w^*) will transform the vector of the partial derivative operators like the basis of a vector space [7]:

$$\frac{\partial}{\partial u^*} = \frac{\partial u}{\partial u^*}\frac{\partial}{\partial u} + \frac{\partial v}{\partial u^*}\frac{\partial}{\partial v} + \frac{\partial w}{\partial u^*}\frac{\partial}{\partial w},$$

$$\frac{\partial}{\partial v^*} = \frac{\partial u}{\partial v^*}\frac{\partial}{\partial u} + \frac{\partial v}{\partial v^*}\frac{\partial}{\partial v} + \frac{\partial w}{\partial v^*}\frac{\partial}{\partial w}, \quad (12)$$

$$\frac{\partial}{\partial w^*} = \frac{\partial u}{\partial w^*}\frac{\partial}{\partial u} + \frac{\partial v}{\partial w^*}\frac{\partial}{\partial v} + \frac{\partial w}{\partial w^*}\frac{\partial}{\partial w},$$

where the transformation matrix may be written as:

$$\partial(u, v, w)/\partial(u^*, v^*, w^*).$$

By this notation, Eqs. (9) can be rewritten as:

$$\begin{pmatrix} A^* \\ U_1^* \\ U_2^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ g_1 & 1 & 0 \\ g_2 & k_2 & 1 \end{pmatrix} \cdot \frac{\partial(r, \varphi, \vartheta)}{\partial(u, v, w)} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \varphi} \\ \frac{\partial}{\partial \vartheta} \end{pmatrix} \quad (13)$$

and the condition for a common solution Eq. (11) becomes

$$\left| \frac{\partial(r, \varphi, \vartheta)}{\partial(u, v, w)} \right| = 0 \quad (14)$$

since the determinant of the first matrix factor is always 1. Again, the condition is independent of the functions g_1, g_2, k_2. Hence, the singularities are introduced into the system by the change of the variables.

Next, the transformation of the differential form, Eq. (5), under Eqs. (8) is considered. The form is represented by its determinant:

$$\mu^* = \begin{vmatrix} \mathrm{d}u & \mathrm{d}v & \mathrm{d}w \\ g_1 & 1 & 0 \\ g_2 & k_2 & 1 \end{vmatrix}.$$

According to the derivation of the Eq. (5), this form should be represented by the determinant:

$$\mu^* = \begin{vmatrix} \mathrm{d}r & \mathrm{d}\varphi & \mathrm{d}\vartheta \\ U_1 r & U_1 \varphi & U_1 \vartheta \\ U_2 r & U_2 \varphi & U_2 \varphi \end{vmatrix}$$

in the new coordinates. The matrix of the determinant may be factorized to give:

$$\mu^* = \begin{vmatrix} \frac{\partial r}{\partial u} & \frac{\partial r}{\partial v} & \frac{\partial r}{\partial w} \\ \frac{\partial \varphi}{\partial u} & \frac{\partial \varphi}{\partial v} & \frac{\partial \varphi}{\partial w} \\ \frac{\partial \vartheta}{\partial u} & \frac{\partial \vartheta}{\partial v} & \frac{\partial \vartheta}{\partial w} \end{vmatrix} \cdot \begin{vmatrix} \mathrm{d}u & \mathrm{d}v & \mathrm{d}w \\ g_1 & 1 & 0 \\ g_2 & k_2 & 1 \end{vmatrix}; \quad (15)$$

Hence, the change of the form μ under the change of variables may be summarized in the equation:

$$\mu^* = \left| \frac{\partial(r, \varphi, \vartheta)}{\partial(u, v, w)} \right| \mu. \quad (16)$$

Note, that the determinant of the Jacobian matrix appears in this expression, which could have singularities according to Equation (14). However, they are just the common solutions.

An Example with Two Variables

The physical significance of the formulas derived so far, may be illustrated by the model of Dreitlein and Smoes [5]. This model is too simple to display all aspects, but permits the verification of some properties and clarifies their meaning. The set of differential equations of the model:

$$\frac{\partial}{\partial t} a_1 = (E - a_1^2 - a_2^2) a_1 + S_1 a_2 - 2 R a_1, \quad (17)$$

$$\frac{\partial}{\partial t} a_2 = (E - a_1^2 - a_2^2) a_2 - S_2 a_1 + 2 R a_2,$$

where a_1, a_2 are time (t) dependent quantities of species and capitals represent time independent parameters; e.g. may be interpreted as the kinetics of a chemical reaction system [5]. By the transformation of a_1, a_2 into the new variables z, Φ:

$$a_1 = z \cdot \cos \Phi, \quad a_2 = a z \cdot \cos(\Phi + \alpha) \quad (18)$$

the Eqs. (17) read:

$$\mathrm{d}\Phi/\mathrm{d}t = S_1 a \cdot \sin \alpha,$$
$$\mathrm{d}z/\mathrm{d}t = [E - z^2(a^2 \cos^2(\Phi + \alpha) + \cos^2 \Phi)] z, \quad (19)$$

$$\text{if} \quad \frac{S_2}{a} - S_1 a = 2(2R - S_1 a \cdot \cos \alpha)$$
$$\cdot \cos \alpha = 0$$

that is:

$$a = \pm S_2/S_1 \quad \text{and} \quad \cos \alpha = \pm 2R/\sqrt{S_1 S_2}.$$

The solution of Eqs. (19) has previously been derived [6]:

$$\Phi = w(t - t_0),$$
$$\left(\exp(2E\,\Phi/w)\right)(e/z^2 - 1 - b \sin(2\Phi + \gamma)) = C,$$

where

$$w = \pm \sqrt{S_1 S_2} \cdot \sin \alpha; \quad e = 2E/(a^2 + 1);$$
$$\gamma = \varepsilon + \delta; \quad \mathrm{tg}\,\delta = E/w;$$
$$\mathrm{tg}\,\varepsilon = (a^2 \sin 2\alpha)/(a^2 \cos 2\alpha + 1);$$
$$d = \sqrt{(S_1 - S_2)^2/(S_1 + S_2)^2 + 16 R^2/(S_1 + S_2)^2} \sin\,\delta,$$

t_0, C are integration constants, and the infinitesimal generator $U_{\Phi z}$ of the corresponding transformation group also:

$$U_{\Phi z} = -\frac{d}{e} z^3 \cos(2\Phi + \gamma) \frac{\partial}{\partial z} + \frac{\partial}{\partial \Phi}. \quad (20)$$

In matrix notation, the generators A and U may be represented in the variables a_1 and a_2 (see (12)) by the inverse transformation of Eqs. (18):

$$\begin{pmatrix} A \\ U \end{pmatrix} = \begin{pmatrix} S_1\, a \sin \alpha & E - z^2(a^2 \cos^2(\Phi + \alpha) + \cos^2 \Phi)\, z \\ 1 & -\dfrac{d}{e} z^3 \cos(2\Phi + \gamma) \end{pmatrix} \cdot \begin{pmatrix} \dfrac{\partial a_1}{\partial \Phi} & \dfrac{\partial a_2}{\partial \Phi} \\ \dfrac{\partial a_1}{\partial z} & \dfrac{\partial a_2}{\partial z} \end{pmatrix} \begin{pmatrix} \dfrac{\partial}{\partial a_1} \\ \dfrac{\partial}{\partial a_2} \end{pmatrix}. \tag{21}$$

The condition of common solutions (Eq. (11)) is determined by the product of the determinants of the matrices:

$$\sigma = a\, z^2 \cdot \left\{ \frac{S_1\, a\, d \sin \alpha}{e} z^2 \cos(2\Phi + \gamma) - E + z^2(a^2 \cos^2(\Phi + a) + \cos^2 \Phi) \right\} \cdot \sin \alpha.$$

After rearranging terms containing cos

$$\sigma = -\, a\, z^2 \{e - z^2(1 + d \sin(2\Phi + \gamma))\} \sin \alpha \tag{22}$$

is obtained. The condition, $\sigma = 0$, gives the singularities of the system as e.g. the limit cycle

$$z^2(1 + d \sin(2\Phi + \gamma)) = e$$

and the unstable point at the origin $z = 0$. However, another aspect is revealed, if the curves $\sigma = 0$ for values of $\cos \alpha = 2\, R / \sqrt{S_1 S_2} > 1$, are examined. In this case, all angles have imaginary values and hence the associated trigonometric functions turn hyperbolic. Hence, besides $z = 0$, also the curves

$$e - z^2(1 + d \sinh(2\Phi + \gamma)) = 0,$$

fulfil the condition $\sigma = 0$. These curves are separatrices which divide the a_1, a_2 plane into domains [8]. The boundaries of the domains are represented by the curves $\sigma = 0$. The singular points of the Eqs. (17) belong to the curves, since $\sigma = 0$ because of zeros in the row for A of the matrix in Equation (21). Also the limit cycle is in this respect a boundary of domains. Since no trajectory intersects a boundary of a domain, they all remain within their respective domain. Within a domain, the sign of σ does not change, i.e. σ remains either positive or negative and becomes only zero at the boundary. Hence, if the system moves along a trajectory, its σ parameter has a definite sign. The form μ of this system is calculated from the determinant of Eq. (20):

$$\mu = \begin{vmatrix} d\Phi & dz \\ 1 & -\dfrac{d}{e} z^3 \cos(2\Phi + \gamma) \end{vmatrix} \tag{23}$$

$$= dz + \frac{d}{e} z^3 \cos(2\Phi + \gamma)\, d\Phi.$$

The integrating factor $-z^{-3}/2$ allows the evaluation of a potential function:

$$-\frac{z^{-3}}{2} \mu = d\left(\frac{1}{z^2} - \frac{d}{e} \sin(2\Phi + \gamma) \right).$$

The curves:

$$\frac{1}{z^2} - \frac{d}{e} \sin(2\Phi + \gamma) = \text{const}$$

are solutions of (20). Therefore, they represent the paths along which the trajectories are transformed
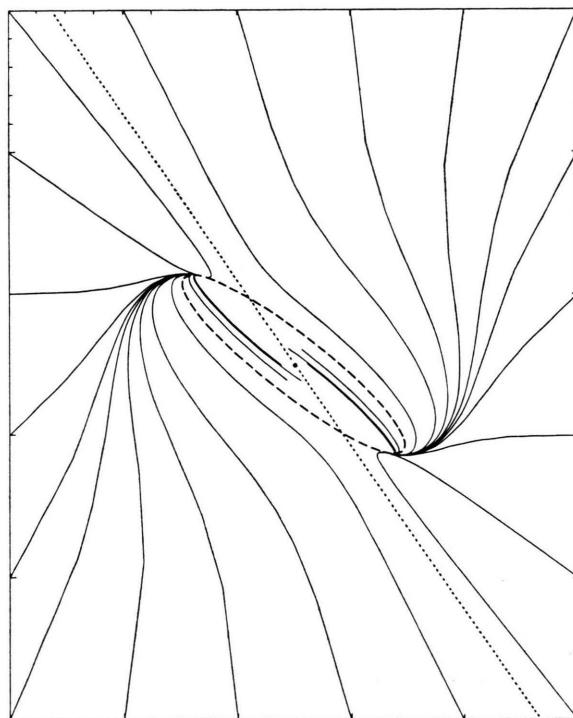

Fig. 1. Family of trajectories of the differential equation system (17), where $E = 1.0$, $R = 1.04$ and $S_1 = S_2 = S = 2.0$. The trajectories are separated by a set of separatrices drawn as dashed lines. The mathematical functions of separatrices are obtained by the condition (Eq. (22)) $\sigma = 0$, where σ is an entropylike function.

into each other by the group generated by Equation (20). Moreover, they furnish the a_1, a_2-plane with a potential function. The potential function and σ display properties which already are well known from thermodynamic functions. Nevertheless, it is necessary to extend the model to the case of three variables, since e.g. μ in the two dimensional planes in contrast to the three dimensional case always possesses an associated potential function.

An Example with Three Variables

The two dimensional models of Dreitlein and Smoes may be extended to three dimensions by transformation of the vector basis $(\partial/\partial r, \partial/\partial\varphi, \partial/\partial\vartheta)$

further and ultimately to $(\partial/\partial a_1, \partial/\partial a_2, \partial/\partial a_3)$. We may as in the two dimensional case, at first use the transformation:

$$\frac{1}{r^2} = \frac{1}{z^2} + f(\Phi, \Theta); \quad \varphi = \Phi; \quad \vartheta = \Theta, \quad (24)$$

where $f(\Phi, \Theta)$ is a not definitely specified function; followed by a generalized transformation of the spherical polar coordinates:

$$\begin{aligned}
a_1 &= z \cos(\Phi) \sin \Theta, \\
a_2 &= a\, z \cos(\Phi + \alpha) \sin \Theta, \quad\quad (25) \\
a_3 &= b\, z \cos(\Theta + \beta).
\end{aligned}$$

The new infinitesimal generators are then obtained by the following transformations (compare Eq. (10))

$$\begin{bmatrix} A \\ U_1 \\ U_2 \end{bmatrix} = G\,C\,\frac{\partial(r, \varphi, \vartheta)}{\partial(u, v, w)}\,\frac{\partial(z, \Phi, \Theta)}{\partial(r, \varphi, \vartheta)}\,\frac{\partial(a_1, a_2, a_3)}{\partial(z, \Phi, \Theta)} \cdot \begin{bmatrix} \dfrac{\partial}{\partial a_1} \\ \dfrac{\partial}{\partial a_2} \\ \dfrac{\partial}{\partial a_3} \end{bmatrix}, \quad (26)$$

where G and C are the first two matrix factors of Equation (10) and

$$\frac{\partial(z, \Phi, \Theta)}{\partial(r, \varphi, \vartheta)} = \begin{pmatrix} \dfrac{z^3}{r^3} & 0 & 0 \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Phi} & 1 & 0 \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Theta} & 0 & 1 \end{pmatrix},$$

$$\frac{\partial(a_1, a_2, a_3)}{\partial(z, \Phi, \Theta)} = \begin{pmatrix} \cos(\Phi)\sin\Theta & a\cos(\Phi+\alpha)\sin\Theta & b\cos(\Theta+\beta) \\ -z\sin\Phi\sin\Theta & -z\,a\sin(\Phi+\alpha)\sin\Theta & 0 \\ z\cos\Phi\cos\Theta & z\cos(\Phi+\alpha)\cos\Theta & -b\,z\sin(\Theta+\beta) \end{pmatrix}.$$

Its determinant is

$$\left| \frac{\partial(a_1, a_2, a_3)}{\partial(z, \Phi, \Theta)} \right| = a\,b\,z^2 \sin\Theta \sin\alpha \cos\beta.$$

Subsequently, from Eq. (26, the condition of the common solution yields the function σ, which of course resembles Eq. (22):

$$\sigma = a\,b\,z^2 \sin\alpha \cos\beta \sin\Theta\,\frac{z^3}{r^3}\,r(r^2 - E)\,K\,S.$$

This function may be recast with the transformation Eq. (24) into

$$\sigma = a\,b\,K\,S\sin\alpha\cos\beta \cdot z^3 \sin\Theta[-E + z^2(1 - E\,f(\Phi, \Theta))]. \quad (27)$$

The condition $\sigma = 0$ leads to:
1. the singularity $z = 0$ at the origin,
2. the condition for the separatrices

$$z^2(1 - E\,f(\Phi, \Theta)) - E = 0,$$

which are surfaces dividing the three dimensional space (a_1, a_2, a_3) into domains and to the condition $\Theta = 0$, which identifies the a_3-axis as a singular line.

Again, the singular points of the generator A in Eq. (26) are situated on the functions $\sigma = 0$, since all components (i.e. a row of the determinant) are zero. In addition, there may be two rows of the matrix equivalent: $A = \lambda_1 U_1$ or $A = \lambda_2 U_2$ for which λ_1 and λ_2 are functions of a_1, a_2 and a_3. In this case, singular solutions are obtained e.g. a limit cycle, which again reside on the graphs given by $\sigma = 0$.

In both cases, the condition $\sigma = 0$ of (22) and (27) divide the space into domains, in which σ has a definite sign, and no trajectory crosses the boundary of its domain. Hence, σ has also entropy-like properties in more-dimensional systems.

It is useful to evaluate the matrix product in (26) to calculate the form μ:

$$\frac{\partial(a_1, a_2, a_3)}{\partial(u, v, w)} = \begin{pmatrix} B \cdot z & -K & -S \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Phi} & 1 & 0 \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Theta} & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \dfrac{a_1}{z} & \dfrac{a_2}{z} & \dfrac{a_3}{z} \\ -a_1 \operatorname{tg}\Phi & a_2 \operatorname{tg}(\Phi + \alpha) & 0 \\ a_1 \operatorname{ctg}\Theta & a_2 \operatorname{ctg}\Theta & a_3 \operatorname{tg}(\Theta + \beta) \end{pmatrix}, \tag{28}$$

where

$$B = -E + z^2(1 - E f - K/2 \cdot \partial f/\partial \Phi - S/2\, \partial f/\partial \Theta).$$

Once more, the form μ will be expressed not as da_1 but in terms of dz, $d\Phi$ and $d\Theta$, since the latter form is more compact and displays the same features as the former:

$$\mu = \begin{vmatrix} dz & d\Phi & d\Theta \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Phi} & 1 & 0 \\ \dfrac{z^3}{2}\dfrac{\partial f}{\partial \Theta} & 0 & 1 \end{vmatrix} = dz - \frac{z^3}{2}\left(\frac{\partial f}{\partial \Phi}\, d\Phi + \frac{\partial f}{\partial \Theta}\, d\Theta\right). \tag{29}$$

The integrating factor, $-2/z^3$, reveals the potential function T:

$$T = 1/z^2 + f,$$

so that (29) reads

$$-\tfrac{1}{2} z^3 \mu = dT.$$

In general, it would not be possible to integrate a 1-form in three variables, since it may not be rendered exact by an integrating factor, while the exact form is always attainable with two variables. Here, the integrability is achieved by setting the arbitrary functions g_1, g_2 of Eq. (5) equal to zero. Then, Eq. (5) takes the simple form of $\mu = du$. Hence, μ can be derived from an exact 1-form and is therefore integrable. The problem of finding a potential function is consequently reduced to that of casting Eq. (5) into an integrable differential form.

The condition of integrability has been developed in the literature [9]. It reads for Eq. (5):

$$0 = \frac{\partial(g_2 - g_1 \cdot k_2)}{\partial v} - \frac{\partial g_1}{\partial w} + g_1 \frac{\partial(g_2 - g_1 \cdot k_2)}{\partial u}$$
$$- (g_2 - g_1 k_2)\frac{\partial g_1}{\partial u}. \tag{30}$$

If Eq. (30) is valid, then Eq. (5) may be written:

$$\mu = \frac{1}{\lambda}(\lambda\, du - \lambda g_1\, dv - \lambda(g_2 - g_1\, k_2)\, dw)$$
$$= \frac{1}{\lambda}\, d\psi, \tag{31}$$

where ψ is the potential function and λ the integrating factor.

Since g_1 and g_2 are unspecified functions, it is always possible to define them so that Eq. (30) is valid. Therefore, it is always possible to define a potential function of the system. Moreover, g_1 and g_2 are not definitively specified by (30). Therefore, the potential function also depends on the choice of g_1 and g_2.

For the sake of completeness, the differential equations for the system in three variables will be given. They may be derived from the generator A of (26) and (28):

$$\frac{da_1}{dt} = B' a_1 + K' a_1 - P a_2/a - S'\frac{a_1 a_3}{b\varrho},$$

$$\frac{da_2}{dt} = B' a_2 - a P a_1 + K' a_2 - S'\frac{a_2 a_3}{b\varrho},$$

$$\frac{da_3}{dt} = B' a_3 - S' b \varrho ,\qquad (32)$$

where

$$\operatorname{tg} \Phi = \frac{-1}{\sin \alpha}\left(\frac{a_2}{a\, a_1} - \cos \alpha\right);$$

$$\operatorname{tg}(\Phi + \alpha) = \frac{1}{\sin \alpha}\left(\frac{a_1\, a}{a_2} - \cos \alpha\right)$$

$$\operatorname{ctg} \Theta = \frac{1}{\cos \beta}\left(\frac{a_3}{b\,\varrho} + \sin \beta\right);$$

$$\operatorname{tg}(\Theta + \beta) = \frac{1}{\cos \beta}\left(\frac{b\,\varrho}{a_3} + \sin \beta\right),$$

$$z^2 = \frac{1}{b^2 \cos^2 \beta}\,(b^2 \varrho^2 + a_3{}^2 + 2 b \sin \beta\, \varrho\, a_3);$$

$$\varrho^2 = \frac{1}{a^2 \sin^2 \alpha}\,(a^2 a_1{}^2 + a_2{}^2 - 2 a \cos \alpha\,(a_1\, a_2)),$$

and where

$$B' = B - S \operatorname{tg} \beta; \quad S' = S/\cos \beta;$$
$$P = K/\sin \alpha; \quad K' = K \cdot \operatorname{ctg} \alpha .$$

The singular points of Eqs. (32) are obtained by equating all time derivatives with zero. An equation system for a_1 and a_2 results when a_3/ϱ of the last equation is inserted in both of the upper Eqs. (32):

$$\begin{pmatrix}0\\0\end{pmatrix} = \begin{pmatrix} B' + K' - (S'^2/B') & -P/a \\ -P \cdot a & B' + K' - (S'^2/B') \end{pmatrix} \cdot \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}.$$

Besides the trivial solution $a_1 = a_2 = 0$, the system also may admit other solutions, if the determinant is zero, i.e.:

$$((B' + K')\, B' - S'^2)^2 = P^2\, B'^2 .\qquad (33)$$

The condition Eq. (33) can be solved for B' since K', S' and P are constant values, hence

$$B = B' + S \operatorname{tg} \beta \quad \text{and}$$
$$[(B' + K')\, B' - S'^2]\, a_1 = P\, B' \cdot a_2 \qquad (34)$$

together with the last equation of (32) form a new equation system in a_1, a_2, a_3. The latter can be solved, if the definite form of B (see (28)) is known. The Eq. (33) is derived here, since it is an essential function in the derivation of the different kinds of networks [2] which are associated with the three variable system. The discriminant of Eq. (33) divides the parameter space in domains which contain the associated families of trajectories.

If the system possesses a singular surface, the latter may be derived from (27), i.e.

$$z^2 (1 - E\, f(\Phi, \Theta)) = E.$$

The limit cycles may be obtained from the conditions $A = \lambda_1 U_1$ and $A = \lambda_2 U_2$ (see the discussion of (27)). The limitation of space precludes the explicit statement of these equations.

Discussion

The examples in two and three variables which are treated here, may be easily be extended to even more variables [9]. In the more-variable systems, functions like σ (Eq. (27)) and μ (Eq. (29)) can be similarly found. However, the transformation from autonomous (see introduction) to time dependent or space-time dependent systems requires additional considerations. The latter extension would be desirable for the elaboration of the theory of thermodynamics of irreversible processes. Here, we shall restrict the discussion to the relation between the properties of σ and μ and of the phenomena known in thermodynamics. At first, the characteristics of σ will be considered.

If the infinitesimal generator A (Eqs. (1)) is written in the form:

$$A = \frac{dx_1}{dt}\frac{\partial}{\partial x_1} + \frac{dx_2}{dt}\frac{\partial}{\partial x_2} + \frac{dx_3}{dt}\frac{\partial}{\partial x_3} + \cdots, \quad (35)$$

where the functions f_i have been replaced by the time derivatives of Eq. (1 a); then the equation for the common solution (see (14)) in three variables reads:

$$\begin{vmatrix} \dfrac{dx_1}{dt} & \dfrac{dx_2}{dt} & \dfrac{dx_3}{dt} \\ u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \end{vmatrix} = \sigma ,$$

where the u_{ij} are the coefficients of the generators of the group of transformations which the generator A admits.

Hence,

$$\sigma = (u_{12}\, u_{23} - u_{22}\, u_{13})\,\frac{dx_1}{dt}$$
$$+ (u_{13}\, u_{21} - u_{11}\, u_{23})\,\frac{dx_2}{dt}$$
$$+ (u_{11}\, v_{22} - u_{21}\, u_{12})\,\frac{dx_3}{dt}$$

is a linear combination in which each term contains a time derivative of a system quantity as a factor. In this form, σ displays a remarkable similarity to the entropy production of thermodynamic systems [10]. The latter is also a sum of products, and each term consists of a factor which is a flow variable and another which is a force. Moreover, σ has during the evolution of the system a definite sign like classical thermodynamic functions (see discussion of Eq. (22)).

Another important function in thermodynamic systems is the energy. The discussion of Eq. (31) has led to the conclusion that the functions g_1 and g_2 may be chosen equal to zero to obtain the potential function u. If Eq. (16) explicitly is written for the generator Eq. (35):

$$X_1 \, dx_1 + X_2 \, dx_2 + X_3 \, dx_3 = \sigma \cdot du , \qquad (37)$$

where X_i are the determinant minors of Eq. (36), then a differential form is obtained, which has the same structure as that for the energy of a closed system. A great variety of systems show the typical properties associated with thermodynamic systems, since the nature of X_j is irrelevant. The main assumption which must be fulfilled by the systems is the validity of the group axioms, inherent in the symmetry transformations of the one-parameter groups, of these the axiom of uniqueness is the most conspicuous. It may be worthwhile to study how the phenomena observed in chaotic systems [11] fit into this concept. A new example must be chosen since the domain boundaries of such systems differ from the ones used here.

Besides the two typical functions σ and u, another aspect is revealed if the network representation of the system is examined. In a previous paper [2], it has been demonstrated, that a variation of the system parameters may cause a dramatic change in the structural organisation of the space of the domains. As long as the parameters are kept constant, the domain structure remains undisturbed, but as soon as the parameters are changed beyond critical limits by an external force, then the domain structure alters and the system may develop along a very different path in time, e.g. before the disturbance it may evolve towards a stationary point (the equilibrium) but afterwards it moves on a limit cycle. Such applications may be of special interest to control economic systems [12]. Remarkable is the local change of the sign of the function σ, which may be accompanied by extensive structural rearrangements in the domains.

Finally, it should be noted, that the laws Eq. (36) and (37) are generated from their simple (canonical) forms, Eq. (5) and (16), by a transformation of the variables. Therefore, the transformation contains the specific information of the system. The laws constituting a system are inherent in the transformation, whereas Eq. (36) and (37) express general properties of the system which already are displayed by the canonical system. The vector space calculus and the group concept of the symmetries found in the transformation groups are examples of such general properties. However, there is still an ambiguity left, since the functions g_1, g_2 and k_2 do not have fixed values. The significance of the ambiguity to real systems has to be explored using realistic examples. The model treated here does not fulfil this requirement. Note, that the function σ has properties of the thermodynamic entropy but is e.g. zero on the limit cycle whereas the entropy is not.

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