

## CONTACT TRANSFORMATIONS AND BRACKETS IN CLASSICAL THERMODYNAMICS\*

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(Received January 29, 1980)

The problem of coordinate transformations in classical equilibrium phenomenological thermodynamics has been solved due to the recognition of the mathematical structure of the space of thermodynamic parameters. Moreover, this structure (contact structure) enables one to introduce, in an intrinsic manner, Lie and semi-Lie algebraic structures to thermodynamics. Three types of brackets are defined which are invariants of any thermodynamically admissible transformation. The role of the so called Legendre transformations considered by Gibbs has been recognized as a special subgroup of contact transformations.

### 1. Introduction

In the development of geometrical theories of equilibrium phenomenological thermodynamics (EPT) one can observe two main lines. One completely developed by Gibbs [11] and the second originated by Carathéodory [7] and developed by Born [4] (cf. also Landé [15]).

In Carathéodory's approach the main stress was put on the formulation of the second law of thermodynamics, i.e., on the well-known *principle of inaccessibility*. This formulation was based on his theorem from the theory of partial differential equations. However, later on mathematicians found his proof to be incomplete and it was even not clear whether this theorem is valid locally or globally. Bernstein [2] and Boyling [5] have proved the global version of this theorem. The main shortcomings of Carathéodory's approach relied on the definition of a thermodynamic space suitable to a given thermodynamic system. According to him it was just a collection of any independent directly measurable thermodynamic parameters which was treated as cartesian coordinates. In such a way the thermodynamic space was not defined uniquely. For one system one can have different independent spaces (e.g. planes  $p$ - $V$  or  $T$ - $V$ ). Moreover, in this approach there is no geometrical distinction between extensive and intensive parameters, what is very important

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\* Supported by Polish Ministry of Science Technology and Higher Education, project MR I. 7.

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for EPT. The main point is, however, that Carathéodory's space does not carry any geometrical structure and for that reason the problem of coordinate transformations in thermodynamics could not be even stated. The necessity of finding a mathematical scheme which would take into account the duality between extensive and intensive parameters and which could also solve the problem of changes of variables in thermodynamics has been already recognized by Ehrenfest [10] in 1911.

The thermodynamic space introduced by Gibbs [11], contrary to Carathéodory's one, is clearly and uniquely defined. This space (widely known as *Gibbs space*) is constituted from  $n+2$  extensive parameters among which  $n$  is independent (one parameter can be eliminated due to the so called homogeneous first-order property of the fundamental relation, see e.g. Callen [6]). Throughout the paper  $n$  is always the same and denotes the number of degrees of freedom for a thermodynamic system. Tisza [23] called this space the *thermodynamic phase space* and Callen [6] *thermodynamic configuration space*, respectively. For the simplest thermodynamic system it was 3-dimensional space with rectangular coordinate axes labelled by volume  $V$ , entropy  $S$  and internal energy  $U$  (if the mole number  $N$  is assumed to be constant). The relation between these three quantities  $U = U(S, V)$  Gibbs called the *fundamental relation* and the surface defined by it the *thermodynamic surface*. Very important feature of Gibbs' approach consists in the fact that it takes into account the distinction between extensive and intensive parameters, namely the extensive parameters form the thermodynamic space while the intensive ones are treated as functions on it (they describe just the slope of the thermodynamic surface). Stability conditions of equilibrium states Gibbs formulated by means of curvature of the thermodynamic surface. In this point, however, his theory although correct dealt with undefined mathematical objects. Namely, it is well known that in Gibbs' space one cannot introduce any Riemannian metric which would have a thermodynamic meaning. Consequently, in this space we are not faced with such fundamental mathematical concepts as distance, orthogonality, and curvature. Of course the notion of curvature one can introduce without metric, namely by means of connection (non-metrical), but this concept has appeared in mathematics already after Gibbs' death. Gibbs' space although very useful has a great disadvantage, namely it does not carry any significant geometrical structure and hence the problem of coordinate transformations in thermodynamics could not be stated in full generality. Later on we will see that the so called *Legendre transformations* regarded by Gibbs stand for the subgroup of the more general group of contact transformations.

In our previous paper [18] and in [19] we have proposed entirely new geometrical formulation of EPT. The central point of these papers consists in the introduction of a new thermodynamic space called a *thermodynamic phase space* (TPS), but not in the sense of that of Tisza [23]. TPS is larger than spaces done by Gibbs and Carathéodory, e.g., if Gibbs' space and Carathéodory's one have dimensions  $n+2$  and  $n$ , respectively, then dimension of TPS is  $2n+1$ . In [18] and [19] we have constructed TPS as *projective fibre bundle* over slightly modified Gibbs space. The modification relies on the replacing extensive parameters by densities. Such procedure reduces dimension of the Gibbs space by one, but it reflects the fact that the properties of any thermodynamic system do not depend

on the overall scale of this system. It is convenient to have a space of higher dimension than the number of degrees of freedom because in such a case equations characteristic for a given physical theory can be interpreted geometrically as some submanifolds of this space. We mean here the so called null submanifolds of maximal dimension commonly called as *Lagrangian* or *Legendre submanifolds*. Consequently analysis of a theory can be replaced by investigation of geometrical properties of such submanifolds (cf., Ślawnowski [21], [22]).

Owing to the concept of TPS the classical thermodynamics has been brought into the formalism similar to that of classical Hamiltonian mechanics (see the sketch below).

| mechanics   | thermodynamics   |
|---|--|
| <div style="border: 1px solid black; padding: 5px;">           Phase space <math>T^*Q</math><br/> <math>w = (p_1, \dots, p_n; q_1, \dots, q_n)</math><br/>           symplectic structure <math>\gamma</math><br/> <math>\gamma = dp_i \wedge dq^i, \gamma^n \neq 0</math> </div> | <div style="border: 1px solid black; padding: 5px;">           Thermodynamic phase space <math>M^{2n+1}</math><br/> <math>m = (p_1, \dots, p_n; x^0, x^1, \dots, x^n) \in M^{2n+1}</math><br/>           contact structure <math>\theta</math><br/> <math>\theta = dx^0 + p_i dx^i, \theta \wedge (d\theta)^n \neq 0</math> </div> |
| $\downarrow \pi$  | $\downarrow \pi$   |
| <div style="border: 1px solid black; padding: 5px;">           Configuration space <math>Q</math><br/> <math>\pi(w) = q = (q^1, \dots, q^n)</math><br/>           metric structure         </div>   | <div style="border: 1px solid black; padding: 5px;">           Modified Gibbs space <math>B^{n+1}</math><br/> <math>\pi(m) = x = (x^0, x^1, \dots, x^n)</math><br/>           no structure         </div>  |

Here  $\gamma$  denotes the Poincaré invariant,  $\theta$ —energy 1-form in thermodynamics,  $\wedge$ —the exterior product,  $d$ —the operation of exterior differentiation and  $(d\theta)^n = d\theta \wedge \dots \wedge d\theta$  ( $n$  times).

As we see from this sketch on TPS we have so called *contact structure* [3] which is in close relation to the *symplectic structure* (occurring in mechanics). Moreover, by means of a *contact form*  $\theta$  we can introduce on TPS Lie algebraic and semi-Lie algebraic structures similarly as in mechanics by means of the symplectic form  $\gamma$ .

The basic mathematical concepts we use here are differentiable manifolds, fibre bundles, exterior differential forms and Lie algebras of vector fields and functions. Through this paper we are confined only to the  $C^\infty$  (smooth) objects.

## 2. Remarks to the second law of thermodynamics

In [18] the second law of thermodynamics has been formulated as Postulate 2., namely

"On TPS there exists a distinguished part  $\psi$  of the energy form  $\theta$  called the heat form. Its rank is equal to two".

Mathematically it means that  $d\psi \wedge \psi = 0$  and consequently from the Darboux theorem [1] we know that on  $M$  there exist local coordinates in terms of which  $\psi$  assumes the form

$$\psi = f dg, \quad f, g: M^{2n+1} \rightarrow \mathbb{R}^1 \quad (1)$$

Bernstein [2] and Boyling [5] showed that functions  $f$  and  $g$  are defined globally on  $M$ : Because  $\theta$  is defined also globally we have:

*Corollary 1:* The heat form  $\psi$  is the 1-form reduced to a 2-dimensional submanifold  $M^2 \subset M^{2n+1}$ , namely to the submanifold on which coordinate lines are defined (globally) by  $f$  and  $g$ ; i.e., for  $\theta$  we have global decomposition  $\theta = \psi + \Omega$  (where  $\Omega$  is defined as  $\Omega = \theta - \psi$ ). From this decomposition we have

*Corollary 2:* Thermodynamic phase space  $M^{2n+1}$  can be globally decomposed into the cartesian product of two submanifolds

$$M^{2n+1} = M_t^2 \times M_d^{2n-1}. \quad (2)$$

These submanifolds of dimensions 2 and  $2n-1$ , respectively, are defined by the decomposition  $\theta = \psi + \Omega$  of the contact form  $\theta$  in the following way. Let us assume that (2) is true and we have canonical projections

$$\pi_t : M^{2n+1} \rightarrow M_t^2, \quad \pi_d : M^{2n+1} \rightarrow M_d^{2n-1}. \quad (3)$$

Let  $\tilde{\psi}$  and  $\tilde{\Omega}$  denote some (linear) forms of maximal ranks defined, respectively, on  $M_t^2$  and  $M_d^{2n-1}$  such that

$$\psi = \pi_t^* \tilde{\psi}, \quad \psi|_{\pi_t^{-1}(q)} = 0, \quad (4)$$

where  $q \in M_t^2$ ,  $\tilde{\psi} \in T^*M_t^2$ ,  $\psi \in T^*M^{2n+1}$ ,  $\pi_t^*$  denotes the pullback of forms and let

$$\Omega = \pi_d^* \tilde{\Omega}, \quad \Omega|_{\pi_d^{-1}(r)} = 0, \quad (5)$$

where  $r \in M_d^{2n-1}$ ,  $\tilde{\Omega} \in T^*M_d^{2n-1}$  and  $\Omega \in T^*M^{2n+1}$ . Assuming  $\theta = \pi_t^* \tilde{\psi} + \pi_d^* \tilde{\Omega}$  we see from (3)–(5) that (2) is satisfied.

Thus we see that the second law which is a central point of thermodynamics is in this formalism equivalent to the decomposition of any thermodynamic space onto the space of the so called *thermal parameters*  $M_t^2$  and the space of the so called *deformation parameters*  $M_d^{2n-1}$  (cf. e.g., [23]).  $\Omega$  can be interpreted within such classical areas of phenomenology as mechanics or electrodynamics, but  $\psi$  can be not.

### 3. Contact transformations of TPS

Introducing in [18] TPS as the projective bundle over slightly modified Gibbs space we distinguished carefully between extensive parameters represented there by densities  $x^0, x^1, \dots, x^n$  and the intensive parameters represented by  $p_1, \dots, p_n$ . But it is no longer necessary. We will no longer distinguish between these two types of parameters as it is often done in practical applications of thermodynamics, where we measure some combinations of “ordinary” thermodynamic parameters. But in this point we face the problem of thermodynamically admissible transformations of variables. Quite recently this problem has been considered, from a similar point of view as here, by Mistura [17].

In our approach the problem of transformations of thermodynamic parameters is solved automatically due to the recognition of the mathematical structure of TPS. As it

was pointed out in [18] TPS carries remarkable geometrical structure, namely, the so called *contact structure*, i.e., structure defined by differentiable linear form  $\theta$  such that  $\theta \wedge (d\theta)^n \neq 0$  [3]. Due to this we can introduce a more general definition of TPS than that of [18].

**Definition 1:** Any  $2n+1$  dimensional manifold  $M$  of all thermodynamic parameters of a physical system on which there exists a contact structure defined by the energy 1-form  $\theta$  will be called the *thermodynamic phase space* of the given system.

Shortly, we will denote TPS as a pair  $(M, \theta)$ , where  $\dim M = 2n+1$  and  $\theta \wedge (d\theta)^n \neq 0$ , or just as  $M$ .

Contact structure of TPS guarantees the full generality of the theory because although it does not offer any special system of coordinates, nevertheless ensures that the coordinates will appear in canonically conjugated pairs, but one. Moreover, because each contact manifold is locally isomorphic to a projective bundle [1], we are always able to find an appropriate transformation from a general TPS to a suitable projective bundle and come back to the "ordinary" thermodynamic parameters. Due to such transformations on TPS, in fact, we have geometrical distinction between extensive and intensive parameters.

Since we have assumed as a primary fact that TPS has a contact structure, the problem of coordinate transformations in thermodynamics can be completely solved, namely, in EPT we are confined only to transformations which preserve the contact structure of TPS, i.e., to the so called *contact transformations*.

**Definition 2:** A diffeomorphism  $\lambda : M \rightarrow M$  preserving the contact structure, i.e., such that

$$\lambda^*\theta = \varrho\theta, \quad (6)$$

with  $\varrho$  being everywhere a nonvanishing function on  $M$  will be called a *contact diffeomorphism*.

Note that  $\varrho\theta \wedge (d(\varrho\theta))^n = \varrho^{n+1}\theta \wedge (d\theta)^n \neq 0$ . The transformations of type (6) preserve the contact distribution and, respectively, its Legendre submanifolds [3], but in general do not preserve the contact form. Automorphisms  $\lambda : M \rightarrow M$  with  $\varrho \equiv 1$  are called the *strict contact transformations*.

Let  $A$  denote the 1-parameter group of contact diffeomorphisms with elements  $\lambda_t$ , depending differentiably on  $t$ . Then  $A$  defines on  $M$  the vector field  $X$  according to the formula

$$(Xf)(m) = \left. \frac{d}{dt} \right|_{t=0} f(\lambda_t(m)), \quad f \in C^\infty(M, \mathbf{R}^1), \quad m \in M. \quad (7)$$

The vector field  $X$  is called the *infinitesimal contact transformation* or the *contact vector field*. According to the definition of the Lie derivative for any contact vector field  $X$  we have

$$\mathcal{L}_X\theta = \tau\theta, \quad (8)$$



where  $\tau_t = \left. \frac{d\varrho_t}{dt} \right|_{t=0}$ ,  $\lambda_t^* \theta = \varrho_t \theta$ ,  $\varrho_t: M \times \mathbf{R}^1 \rightarrow \mathbf{R}^1$  and  $\lambda_t$  and  $X$  are related by (7). Consequently if  $X$  is a strict vector field we have (from  $\varrho_t \equiv 1$  results  $\tau_t \equiv 0$ )

$$\mathcal{L}_X \theta = 0. \quad (9)$$

Let us now examine, from this general point of view, the transformations introduced to thermodynamics by Gibbs and called in standard textbooks as the Legendre transformations [6]. They form a subgroup of strict contact transformations described locally by  $2n+1$  equations

$$\left. \begin{aligned} z &= x^0 - \phi(p_i, x^i), \\ f_j &= f_j(p_i, x^i), \quad g_j = g_j(p_i, x^i) \end{aligned} \right\} \quad i, j = 1, \dots, n. \quad (10)$$

From  $dz + f_j dg_j = dx^0 + p_i dx^i$  results that

$$\frac{\partial \phi}{\partial x^i} + f_j \frac{\partial g_j}{\partial x^i} = p_i, \quad -\frac{\partial \phi}{\partial p_i} + f_j \frac{\partial g_j}{\partial p_i} = 0. \quad (11)$$

But these formulas one can find in every standard textbook of classical mechanics. They are just conditions that

$$f_j = f_j(p_i, x^i), \quad g_j = g_j(p_i, x^i), \quad i, j = 1, \dots, n \quad (12)$$

are canonical transformations in  $2n$  coordinates with  $\phi(p_i, x^i)$  as *generating function*.

Thus we see that in thermodynamics we use only a subgroup of the full contact group. Hence a possibility appears of introducing much more general transformations of thermodynamic variables and also of introducing quite new thermodynamic potentials in addition to those considered by Gibbs.

The notion of a strict contact vector field enables us to give a formal geometric definition of a quasistatic process.

*Definition 3:* A 1-parameter group of special contact transformations of TPS whose generators fulfill (9) will be called a *quasistatic process*.

Remember that in phenomenological thermodynamics a quasi-static process is defined as a one which can be described by differential 1-form.

#### 4. Lie and semi-Lie algebraic structures on TPS

The symplectic structure of mechanical phase space enables one to introduce the Lie algebra structure (Poisson bracket) in the space of real-valued differentiable functions on the phase space. Similarly, the contact structure of TPS enables us to introduce counterparts of the usual Poisson bracket for real-valued functions on TPS. But because the contact form is a linear form (the symplectic form is bilinear), we can introduce at least three different types of brackets which reduce to the standard Poisson bracket in  $2n$  variables if we project them to  $2n$ -dimensional space with natural symplectic structure defined by the 2-form  $d\theta$  (i.e., to the space defined by  $x^0 = \text{const.}$ , see below).

Such brackets are a very useful tool to verify whether any transformation is a contact or not [12].

First let us quote the following result [20].

*Theorem 1:* The set of all contact vector fields on  $(M, \theta)$  constitutes the Lie algebra with respect to the usual bracket operation.

*Proof:* Let  $X$  and  $Y$  be two contact vector fields and let

$$\mathcal{L}_X \theta = \tau \theta, \quad \mathcal{L}_Y \theta = \sigma \theta.$$

Then

$$\mathcal{L}_{[X,Y]} \theta = [\mathcal{L}_X, \mathcal{L}_Y] \theta = \mathcal{L}_X(\sigma \theta) - \mathcal{L}_Y(\tau \theta) = (\mathcal{L}_X \sigma - \mathcal{L}_Y \tau) \theta.$$

In order to introduce Lie or quasi-Lie algebraic structures in the space of real-valued functions on  $M$  we have yet to introduce the concepts of two remarkable types of vector fields on  $M$ .

A contact form  $\theta$  defines on  $M$   $2n$ -dimensional *distribution*  $D$  by setting

$$D_m = \{X \in T_m M | \theta(X) = 0\}, \quad (13)$$

where  $X$  is a vector field on  $M$ , not necessarily a contact. Because of  $\theta \wedge (d\theta)^n \neq 0$  there exists on  $M$  1-dimensional distribution dual to  $D$ . Such distribution is determined by vector field  $\xi$  such that

$$\theta(\xi) = 1, \quad d\theta(\xi, X) = 0, \quad (14)$$

for all vector fields  $X$  on  $M$ . Moreover for  $M$  orientable  $\xi$  is defined globally. We call  $\xi$  the *characteristic vector field* of the given contact structure. From (14) follows immediately that

$$\mathcal{L}_\xi \theta = 0 \quad \text{and} \quad \mathcal{L}_\xi d\theta = 0, \quad (15)$$

i.e.,  $\theta$  and  $d\theta$  are invariant under the action of the 1-parameter group generated by  $\xi$ . Therefore,  $\xi$  generates the 1-parameter group of strict contact transformations. Remember that  $\mathcal{L}_X \omega = d(\underline{X}|\omega) + \underline{X}|d\omega$  for any differentiable form  $\omega$  and  $\underline{X}|\omega$  denotes the interior product of  $\omega$  by vector field  $X$ . Introducing in  $M$  local canonical coordinates (cf. [18])

$$x^0, x^1, \dots, x^n; p_1, \dots, p_n \quad (16)$$

we have

$$\xi = \frac{\partial}{\partial x^0}. \quad (17)$$

**Remark:** Notice that the characteristic vector field was already introduced by Cartan [9], where his  $\{f\}$  defined by  $(d\theta)^n \wedge df = \{f\} \theta \wedge (d\theta)^n$  is equivalent to our  $\xi f$ .

On symplectic manifolds each real-valued function (Hamiltonian) gives rise to the so called symplectic (Hamiltonian) vector field. We wish to have a similar situation for contact manifolds.

Let  $f$  and  $g$  denote real-valued functions on  $M$ . Let  $\bar{X}_f$  denote the vector field associated with  $f$  defined by

$$\bar{X}_f(g)\theta \wedge (d\theta)^n = dg \wedge df \wedge \theta \wedge (d\theta)^{n-1}. \quad (18)$$

In canonical coordinates (16)

$$\bar{X}_f = p_i \frac{\partial f}{\partial p_i} \frac{\partial}{\partial x^0} - \frac{\partial f}{\partial p_i} \frac{\partial}{\partial x^i} + \left( \frac{\partial f}{\partial x^i} - p_i \frac{\partial f}{\partial x^0} \right) \frac{\partial}{\partial p_i}, \quad (19)$$

$\bar{X}_f$  is not the contact field because

$$\mathcal{L}_{\bar{X}_f}\theta = -(\xi f)\theta + df \neq \theta \quad (20)$$

as we can easily prove e.g. by means of coordinates.

*Lemma:*  $\mathcal{L}_{f\xi}\theta = df$ .

*Proof:*  $\mathcal{L}_{f\xi}\theta = f\mathcal{L}_\xi\theta + df \wedge \xi\lrcorner\theta = df$ . We have used here (15), (14) and the property  $\omega \wedge f = f\omega$  for exterior product of a form  $\omega$  and a function  $f$ .

According to (20) and the above Lemma we are already able to adjust to each function  $f$  the appropriate contact field, namely

$$(\xi f)\theta = df - \mathcal{L}_{\bar{X}_f}\theta = (\mathcal{L}_{f\xi} - \mathcal{L}_{\bar{X}_f})\theta = \mathcal{L}_{X_f}\theta,$$

where

$$X_f = f\xi - \bar{X}_f. \quad (21)$$

$X_f$  will be called the *contact vector field* related to the *contact Hamiltonian*  $f$ . In coordinates (16) we have

$$X_f = \left( f - p_i \frac{\partial f}{\partial p_i} \right) \frac{\partial}{\partial x^0} + \frac{\partial f}{\partial p_i} \frac{\partial}{\partial x^i} - \left( \frac{\partial f}{\partial x^i} - p_i \frac{\partial f}{\partial x^0} \right) \frac{\partial}{\partial p_i}. \quad (22)$$

*Remark:* For another construction of  $X_f$  see Kobayashi [14] or Hatakeyama [13].

Notice that  $\theta(X_f) = f$  while  $\theta(\bar{X}_f) = 0$ .

Having  $\theta$ ,  $\xi$ ,  $\bar{X}_f$  and  $X_f$  we will introduce now, one after the other, three types of brackets on  $M$ .

*Definition 4.* Let  $f, g$  denote two contact Hamiltonians on  $M$ . The *Poisson bracket*  $\{f, g\}$  of  $f$  and  $g$  we will call the contact Hamiltonian associated to contact vector field  $[X_f, X_g]$ , i.e.,

$$\{f, g\} = \theta([X_f, X_g]). \quad (23)$$

In coordinates (16)

$$\{f, g\} = \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^i} - \frac{\partial f}{\partial x^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial x^0} \left( g - p_i \frac{\partial g}{\partial p_i} \right) + \frac{\partial g}{\partial x^0} \left( f - p_i \frac{\partial f}{\partial p_i} \right). \quad (24)$$



From the definition (23) we immediately obtain the following properties for this bracket:

P1. antisymmetry,  $\{f, g\} = -\{g, f\}$ ,

P2. bilinearity,  $\{f, \alpha g_1 + \beta g_2\} = \alpha \{f, g_1\} + \beta \{f, g_2\}$ ,  $\alpha, \beta \in \mathbf{R}^1$ ,

P3. Jacobi's identity  $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ ,  $f, g, h \in C^\infty(M)$ .

Moreover, by means of coordinates it can be proved that  $\{f, g\}$  can be defined as

P4.  $\{f, g\} = X_f(g - \xi(f)g)$ .

From P1. to P3. we see that the Poisson bracket introduces the Lie algebraic structure in the space of  $C^\infty$  functions on  $M$ . For canonical coordinates we have

$$\begin{aligned} \{x^0, x^l\} &= -x^l, & \{x^0, p_l\} &= 0, & \{x^l, x^k\} &= 0 \\ \{p_l, p_k\} &= 0, & \{x^l, p_k\} &= -\delta_k^l. \end{aligned} \quad (25)$$

*Definition 5.* The Cartan bracket  $[f, g]$  of  $f, g \in C^\infty(M)$  we define as

$$[f, g] = \bar{X}_f(g). \quad (26)$$

In coordinates

$$[f, g] = \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^i} - \frac{\partial f}{\partial x^i} \frac{\partial g}{\partial p_i} + p_i \left( \frac{\partial f}{\partial x^0} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^0} \right). \quad (27)$$

Remark: From the definition of  $\bar{X}_f$  (18) immediately results equivalent definition of  $[f, g]$ , namely

$$[f, g]\theta \wedge (d\theta)^n = dg \wedge df \wedge \theta \wedge (d\theta)^{n-1}. \quad (28)$$

This type of bracket we call "Cartan bracket" because in the invariant form (28) it has been for the first time introduced by Cartan [9]. Carathéodory called it "die eckige Klammer" [8]. Properties of this bracket are as follows:

C1. antisymmetry, results from (28),

C2. bilinearity, results from (28),

C3.  $[f, [g, h]] + [g, [h, f]] + [h, [f, g]] = \xi(f)[g, h] + \xi(g)[h, f] + \xi(h)[f, g]$  (cf. [8], or [16]).

Bracket  $[f, g]$  can be also defined alternatively as

C4.  $[f, g] = f\xi(g) - X_f(g)$ , or

C5.  $[f, g] = d\theta(X_g, X_f)$ .

The property C4. results immediately from the definition of  $X_f$  while C5. results from the relations  $\mathcal{L}_X\theta = d(X|\theta) + X|\theta$ ,  $\mathcal{L}_{X_g}\theta = (\xi(g)\theta)$  and from C4., namely

$$\begin{aligned} d\theta(X_g, X_f) &= (X_g|\theta)(X_f) = (\mathcal{L}_{X_g}\theta - d(X_g|\theta))(X_f) \\ &= (\xi(g)\theta - dg)(X_f) = f\xi(g) - X_f(g). \end{aligned}$$

For canonical coordinates

$$\begin{aligned} [x^0, x^l] &= 0, & [x^0, p_l] &= -p_l, & [x^l, x^k] &= 0, \\ [p_k, p_l] &= 0, & [x^l, p_k] &= \delta_k^l. \end{aligned} \quad (29)$$

Relation between these two brackets has the form

$$\{f, g\} = f\xi(g) - g\xi(f) - [f, g]. \quad (30)$$

*Definition 6.* The *Lagrange bracket*  $(f, g)$  we define as

$$(f, g) = X_f(g). \quad (31)$$

In coordinates

$$(f, g) = \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^i} - \frac{\partial f}{\partial x^i} \frac{\partial g}{\partial p_i} + p_i \left( \frac{\partial f}{\partial x^0} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x^0} \right) + f \frac{\partial g}{\partial x^0}. \quad (32)$$

This bracket is not antisymmetric. But instead of skew-symmetry we have (from the definitions of  $X_f$  and  $\bar{X}_f$ )

$$L1. (f, g) + (g, f) = f\xi(g) + g\xi(f).$$

The next properties are

L2. bilinearity,

$$L3. (f, g) = \{f, g\} + \xi(f)g, \quad \text{from P4.},$$

$$L4. (f, g) = f\xi(g) - [f, g], \quad \text{from C4.}$$

For canonical coordinates

$$\begin{aligned} (x^0, x^l) &= 0, & (x^l, x^0) &= x^l, & (x^0, p_l) &= p_l, & (p_l, x^0) &= -p_l, \\ (x^l, x^k) &= (x^k, x^l) &= 0, & (p_l, p_k) &= (p_k, p_l) &= 0, \\ (x^l, p_k) &= -\delta_k^l, & (p_k, x^l) &= \delta_k^l. \end{aligned} \quad (33)$$

Bracket  $(f, g)$  is not skew-symmetric and hence we have to write two times more relations as for two foregoing cases.

If we restrict ourselves only to functions  $f, g$  for which  $\xi(f) = \xi(g) \equiv 0$ , then the three types of brackets reduce (within the sign) to the usual Poisson bracket in  $2n$  variables  $(p_i, x^i)$ . It is obvious because in each contact manifold a structure of a 1-dimensional fibre bundle [20] can be introduced. We have already stated that integral curves of the field  $\xi$  for orientable contact manifolds are defined globally. If we assume these curves as fibres and introduce in  $M$  an equivalence relation  $\sim$  such that two points  $m_1, m_2 \in M$  are in relation,  $m_1 \sim m_2$  if and only if  $m_1$  and  $m_2$  belong to the same fibre, then the quotient space  $M/\sim$  can be treated as the base space of the mentioned fibre bundle, and, moreover, it bears symplectic structure induced by the contact structure on  $M$ .

These three types of brackets stand for the very convenient tool in order to prove whether any transformation of thermodynamical variables is admissible or not, i.e., to prove whether it is contact transformation or not. This is due to the following theorem.

*Theorem 2.* If  $\lambda: M \rightarrow M$  is a contact diffeomorphism such that  $\lambda^*\theta = q\theta$  and  $f$  and  $g$  are functions on  $M$  such that  $\lambda^*f = F$  and  $\lambda^*g = G$  then for all types of brackets we have

$$|F, G| = q^{-1}|f, g|, \quad (34)$$

where  $|\cdot, \cdot|$  denotes symbolically the three types of brackets.

**Proof:** Let  $\lambda_*$  denote the induced by  $\lambda$  transformation of vector fields tangent to  $M$ . Then from (14) we see that  $\lambda_*\xi = q^{-1}\xi$ . Similarly, from (18)  $\lambda_*\bar{X}_f = q^{-1}\bar{X}_f$  and consequently from (21)  $\lambda_*X_f = q^{-1}X_f$ . Now (34) follows immediately from P4., (26) and (31).

**Corollary:** All three brackets are invariant under the strict contact transformations.

Thus in thermodynamics we are confined only to such changes of parameters which preserve the above three types of brackets up to a multiplicative function.

**Remark:** Formula (34) has been proved in local coordinates by Carathéodory [8] for the Poisson and Cartan brackets. The more complicated proof for the Cartan bracket can be also found in [12].

To this end let us stress that the above three types of brackets are defined here by means of the contact form  $\theta$  only, without any reference to even dimensional spaces (symplectization of a contact manifold) as was done in [1] or [8].

I am indebted to Professor R. S. Ingarden for his critical permanent interest in this work.

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