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Structure group $U(n) \times 1$ in thermodynamics

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Abstract
In the context of contact geometry, we investigate one aspect of the symmetry of thermodynamics. If with a thermodynamic system with n degrees of freedom we associate a $(2n+1)$-dimensional thermodynamic phase space then we show that the structure group of its tangent bundle can be reduced to the group $U(n) \times 1$.

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1. Introduction

Geometric aspects have always played an important role in the development of every physical theory. Classical mechanics, electrodynamics and, first of all, special and general relativity provide the most prominent examples of such physical theories. Also thermodynamics since the works of Gibbs owed much to geometry. In fact, the first papers of Gibbs dealt with geometric formulation of thermodynamics. The ideas of Gibbs are presented in excellent books by Callen [1, 2]. The underlying concepts in Gibbs' approach are now called the *Gibbs space* and *fundamental relation*. It is well known that for a fluid thermodynamic system having n degrees of freedom, the Gibbs space (GS) is an open region in $\mathbb{R}^{n+1}$ with standard coordinates $U, S, V, N, \ldots$ denoting internal energy, entropy, volume, number of particles and so on. The states of thermodynamic systems are then represented by n-dimensional surfaces given either as $U = U(S, V, N, \ldots)$ or as $S = S(U, V, N, \ldots)$ or as $G = G(T, P, N, \ldots)$ etc, i.e. in the *energy*, *entropy*, *Gibbs potential*, *etc representations*. In differential form these relations are given as $\mathrm{d}U = T\,\mathrm{d}S - P\,\mathrm{d}V + \mu\,\mathrm{d}N + \cdots$, or $\mathrm{d}S = \frac{1}{T}\,\mathrm{d}U + \frac{P}{T}\,\mathrm{d}V - \frac{\mu}{T}\,\mathrm{d}N + \cdots$ or as $\mathrm{d}G = -S\,\mathrm{d}T + V\,\mathrm{d}P + \mu\,\mathrm{d}N + \cdots$, etc. As usual T denotes absolute temperature, P pressure, μ chemical potential, etc; geometrically they describe the slope of tangent planes to the surface of states. Of course, other representations can also be used, and in fact they may be more convenient in particular cases than the energy or entropy representation. Legendre transformations provide one class of representations (or potentials) connected to the energy representation and another class of representations connected to the entropy representation.

Unfortunately, neither classes of potentials are connected by Legendre transformations, although they are connected by more general contact transformations.

However, the problem was that GS had no distinguished geometrical structure. This made it impossible, for instance, to define specific vector fields or brackets of functions on GS, or to find the most general group of symmetries of thermodynamics. The formulation of classical thermodynamics was for a long time not comparable with the symplectic formulation of classical mechanics [3, 4].

Hermann in 1973 [5] proposed to formulate thermodynamics in the framework of *contact geometry* which is an odd-dimensional counterpart of symplectic geometry. This idea was developed in [6] and in many other papers, see e.g. [7]. The approach based on contact geometry proved to be very fruitful for thermodynamics. In general terms, to make the situation in thermodynamics similar to that in mechanics, one needs the notion of the so-called *thermodynamic phase space* (TPS). Roughly speaking, for a thermodynamic system having n degrees of freedom, TPS is a $(2n+1)$-dimensional manifold endowed with a contact structure defined by the *Gibbs 1-form* θ, see [8] and the references therein. As a contact form one can chose $\theta^U = \mathrm{d}U - T\,\mathrm{d}S + P\,\mathrm{d}V - \mu\,\mathrm{d}N + \cdots$ or $\theta^S = \mathrm{d}S - \frac{1}{T}\,\mathrm{d}U - \frac{P}{T}\,\mathrm{d}V + \frac{\mu}{T}\,\mathrm{d}N + \cdots$ or any other differential 1-form of this type, but in each of them all the $2n+1$ thermodynamic parameters are treated as independent. Because of this all these forms are non-degenerate on TPS and define on it the so-called contact structure (see the next section).

The contact structure of TPS allows us to construct thermodynamic theory in a way similar in many respects to analytical mechanics. First of all it allows us to find the most general group of symmetries of classical thermodynamics and go beyond Legendre transformations. This group is the *group of contact transformations* [3, 4]; it is a counterpart of the symplectic group used in analytical mechanics but acting on an odd-dimensional space. Let us mention here that the well-known Legendre transformations form a subgroup of the group of contact transformations. Further, the contact structure of TPS allows one to associate a vector field X_f with any smooth function (contact Hamiltonian) f on TPS. The set of all X_fs forms a Lie algebra. Each vector field X_f generates a 1-parameter group of continuous transformations of TPS (a flow on TPS), and thus represents a continuous symmetry of the thermodynamic formalism. For special choices of f, the flows associated with X_f can even represent various thermodynamic processes. For quite arbitrary (but smooth) functions f, the flows associated with X_f map (deform) some thermodynamic surfaces into other thermodynamic surfaces and thus establish a correspondence between states for different systems. A few examples of f and X_f are given in section 3. For a more detailed analysis of this topic and for more examples of X_fs and their integral curves we refer the reader to [8–11].

The contact structure of TPS also allows us to introduce Riemannian or pseudo-Riemannian metrics on TPS [8, 12] in a sense compatible with the contact structure. Two examples of metrics are given in section 4. So far the meaning of these metrics on the whole $(2n+1)$-dimensional TPS is not quite clear; however one of them, if reduced to n-dimensional thermodynamic surfaces (Legendre submanifolds) given by equation $\theta = 0$ appears to be equivalent to thermodynamic metrics considered by many authors for more than 30 years.

In section 2 we discuss some facts about contact geometry in the form to be used in section 4 which contains the main result of the paper.

2. Contact manifolds

In this section we present briefly a few basic facts about contact geometry [3, 4, 13, 14].

Definition 1. *A differentiable* $(2n+1)$*-dimensional manifold* M *is said to be a contact manifold if it carries a global differential 1-form* θ *such that*

$$\theta \wedge (\mathrm{d}\theta)^n \neq 0, \tag{1}$$

θ *is called the contact form.*

Here $\wedge$ denotes the exterior product, i.e. antisymmetrized tensor product defined as $\mathrm{d}f \wedge \mathrm{d}g = (1/2)(\mathrm{d}f \otimes \mathrm{d}g - \mathrm{d}g \otimes \mathrm{d}f)$, and

$$(\mathrm{d}\theta)^n = \mathrm{d}\theta \wedge \cdots \wedge \mathrm{d}\theta \qquad (n \text{ times}). \tag{2}$$

Condition (1) means that θ is non-degenerate. According to the Darboux theorem [3, 14] this means that there exist on M $2n+1$ local canonical (or contact) coordinates

$$x^0; p_1, \ldots, p_n; x^1, \ldots, x^n \tag{3}$$

in which θ has the simplest (canonical) form

$$\theta = \mathrm{d}x^0 + p_i\, \mathrm{d}x^i, \qquad i = 1, \ldots, n. \tag{4}$$

From now on we shall use the summation convention, i.e. summation over repeated indices. Condition (1), meaning that θ is non-degenerate, can be geometrically interpreted in several ways. The simplest and the most obvious one tells that $\Omega := \theta \wedge (\mathrm{d}\theta)^n$ is proportional to the volume form on M (it should not be confused with the physical volume V occurring in θ^U or θ^S).

Another consequence of condition (1) is that the 1-form θ defines on M two remarkable complementary distributions, i.e. two different fields of tangent planes of dimensions smaller than $2n+1$, or two different subbundles over M of the tangent bundle TM. The existence of these distributions is crucial for this paper.

The first one is the $2n$-dimensional distribution D, i.e. a field of tangent $2n$-dimensional hyperplanes D_x such that

$$D = \bigcup_{x \in M} D_x, \qquad D_x = \{X \in T_x M : \theta(X) = 0\}, \tag{5}$$

where X denotes a vector field on M and $T_x M$ is the tangent space to M at the point $x \in M$. In other words, the distribution D is defined by the kernel $\ker\theta$ of the form θ. This distribution is also called a $2n$-plane bundle. Locally, D can be given by $2n$ vector fields, e.g. by [8]

$$\mathcal{P}_k = \partial/\partial p_k, \qquad \mathcal{X}_k = \partial/\partial x^k - p_k \partial/\partial x^0, \qquad k = 1, \ldots, n. \tag{6}$$

It is obvious from (4) that $\mathcal{P}_k$ and $\mathcal{X}_k$ annihilate θ. The distribution D is usually called a *contact distribution* or a *contact structure* on M [3, 14].

Let us remark that the contact structure D is not given by a unique 1-form θ. If τ is a non-vanishing function on M, then the 1-form $\tau\theta$ also satisfies condition (1) because

$$\tau\theta \wedge (\mathrm{d}(\tau\theta))^n = \tau^{n+1}\theta \wedge (\mathrm{d}\theta)^n \neq 0, \tag{7}$$

and defines the same field D of tangent hyperplanes. Because of this some authors define contact structure in terms of a non-degenerate field of tangent hyperplanes rather than in terms of θ; for details see e.g. [3].

The second distribution, in a sense dual to the first one, is the one-dimensional *characteristic distribution* Ξ defined by a global *characteristic vector field* ξ such that

$$i_\xi\, \mathrm{d}\theta = 0, \qquad i_\xi\theta \equiv \theta(\xi) = 1, \tag{8}$$

or equivalently $i_\xi(\theta \wedge (\mathrm{d}\theta)^n) = (\mathrm{d}\theta)^n$, where i_ξ denotes the internal product (contraction) (of θ and $\mathrm{d}\theta$) with ξ. Thus Ξ is defined by $\ker \mathrm{d}\theta$, i.e. the kernel of $\mathrm{d}\theta$. The condition $i_\xi\theta = 1$ means only normalization of ξ. In the contact coordinates (3)

$$\xi = \partial/\partial x^0. \tag{9}$$

Thus, $TM = D \oplus \Xi = \ker\theta \oplus \ker \mathrm{d}\theta$, where, as it was mentioned above, D and Ξ are two complementary vector subbundles of TM (summation is fibrewise, i.e. $T_xM = D_x \oplus \Xi_x$, $x \in M$).

The fields (6) and (9) satisfy the following commutation relations [8]:

$$[\mathcal{X}_i, \mathcal{X}_j] = [\mathcal{P}_i, \mathcal{P}_j] = [\mathcal{X}_i, \xi] = [\mathcal{P}_i, \xi] = 0, \qquad [\mathcal{X}_i, \mathcal{P}_j] = \delta_{ij}\xi. \tag{10}$$

The last of these commutators shows that the distribution D is not involutive; and this is another geometrical aspect of condition (1). The fact that D is not involutive means that the contact distribution is not maximally integrable, i.e. the field of tangent hyperplanes D does not have $2n$-dimensional integral manifolds. Actually, condition (1) means that the field D is maximally non-integrable [3], i.e. the maximal dimension of integral manifolds of D (or, equivalently, integral manifolds of equation $\theta = 0$) is n.

The existence of n-dimensional integral (sub)manifolds is guaranteed because they may be given for instance by $n+1$ equations $x^i = C^i$, $i = 0, 1, \dots, n$, where C^i are arbitrary constants, or by $n+1$ equations

$$x^0 = \phi(x^1, \dots, x^n), \qquad p_i = -\frac{\partial\phi(x^1, \dots, x^n)}{\partial x^i}, \qquad i = 1, \dots, n. \tag{11}$$

In the first of these equations one recognizes the most standard form of fundamental relation, and *equations of state* in the remaining equations [1, 2].

More generally, one can easily prove [3, 8] that for any partition $I \cup J$ of the set of indices $\{1, \dots, n\}$ into two disjoint subsets I and J, and for a function $\phi(p_I, x^J)$ of n variables $\{p_i, x^j\}$, $i \in I$, $j \in J$, the $n+1$ equations

$$x^0 = \phi - p_i\frac{\partial\phi}{\partial p_i}, \qquad p_j = -\frac{\partial\phi}{\partial x^j}, \qquad x^i = \frac{\partial\phi}{\partial p_i} \tag{12}$$

define a Legendre submanifold in M^{2n+1}. (Legendre submanifolds will be denoted by $\mathcal{S}$.) Conversely, every Legendre submanifold of (M^{2n+1}, θ) in a neighbourhood of any point is defined by these equations for at least one of the 2^n possible choices of the subset I. In equations (12) one recognizes the fundamental relation, equations of state and Legendre transforms. These equations for Legendre (sub)manifolds can be used e.g. in the process of reducing Riemannian metrics from the full TPS to the so-called thermodynamic surfaces.

3. Contact transformations of TPS

Of primary interest for this paper is the group Λ of diffeomorphisms of M which preserve its contact structure. Apart from discrete transformations we can also consider continuous diffeomorphisms as well as their infinitesimal counterparts, i.e. vector fields (generators) associated with these diffeomorphisms.

Definition 2. *A diffeomorphism $\lambda : M \to M$ is said to be a contact diffeomorphism if it preserves the contact distribution D of M, i.e. λ is such that*

$$\lambda^*\theta = \rho\theta, \qquad \lambda \in \Lambda, \tag{13}$$

where ρ is a non-vanishing function on M and λ^* is the pull-back map [15] induced by λ.

Note that the new transformed form $\lambda^*\theta$ is a contact form; it is also non-degenerate because $\rho\theta \wedge (\mathrm{d}(\rho\theta))^n = \rho^{n+1}\theta \wedge (\mathrm{d}\theta)^n \neq 0$. Thus λ preserves the contact structure but does not preserve the contact form. Diffeomorphisms with $\rho = 1$ preserve also the contact form and are called *strict contact transformations*.

Analogously, by a 1-parameter group of *continuous contact transformations* we mean a subgroup of mappings $\lambda_t : M \to M$ of Λ which preserve the contact distribution D, i.e. λ_t are such that

$$\lambda_t^* \theta = \rho_t \theta, \qquad \lambda_t \in \Lambda, \tag{14}$$

where again ρ_t is a non-vanishing function on M.

Let X be a generator of this 1-parameter subgroup of Λ, that is X is in the standard way defined by the formula

$$(XF)(m) = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \lambda_t^* F(m) \equiv \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F(\lambda_t(m)), \qquad \forall m \in M, \tag{15}$$

for any smooth function F on M. Hence X is a vector field whose flow is given by λ_t.

First we shall consider examples of continuous transformations of (M^{2n+1}, θ). For this we need the concept of contact vector field X_f, and its associated flow, corresponding to a smooth function f on M^{2n+1}.

Definition 3. *By a contact vector field associated with a function f on M^{2n+1} we mean a vector field X_f defined by two conditions:*

$$i_{X_f}\theta \equiv \theta(X_f) = f, \qquad i_{X_f}\,\mathrm{d}\theta = -\mathrm{d}f + (\xi f)\theta. \tag{16}$$

It is easy to check that in the standard contact coordinates (3) X_f takes the form

$$X_f = \left(f - p_i \frac{\partial f}{\partial p_i}\right)\frac{\partial}{\partial x^0} + \left(p_i \frac{\partial f}{\partial x^0} - \frac{\partial f}{\partial x^i}\right)\frac{\partial}{\partial p_i} + \frac{\partial f}{\partial p_i}\frac{\partial}{\partial x^i}. \tag{17}$$

Because general form of any vector field on M^{2n+1} is

$$X = \dot{x}^0 \frac{\partial}{\partial x^0} + \dot{p}_i \frac{\partial}{\partial p_i} + \dot{x}^i \frac{\partial}{\partial x^i}, \tag{18}$$

thus, comparing the last two expressions, for the components of X_f we have

$$\dot{x}^0 = f - p_i \frac{\partial f}{\partial p_i}, \qquad \dot{p}_i = p_i \frac{\partial f}{\partial x^0} - \frac{\partial f}{\partial x^i}, \qquad \dot{x}^i = \frac{\partial f}{\partial p_i}. \tag{19}$$

Incidentally, for a constant function $f = 1$, $X_1 = \xi$. One can see that the field X_f is quite complicated, but if we 'cut' x^0 and thus reduce M^{2n+1} to M^{2n} then (19) reduces to

$$\dot{p}_i = -\frac{\partial f}{\partial x^i}, \qquad \dot{x}^i = \frac{\partial f}{\partial p_i}. \tag{20}$$

The last field is well known in classical mechanics as the Hamiltonian vector field corresponding to a Hamiltonian $f : M^{2n} \to \mathbb{R}$. Because of this $f : M^{2n+1} \to \mathbb{R}$ is called a *contact Hamiltonian* and X_f is called a *contact (Hamiltonian) vector field*.

Now we give examples of f of two types. In examples 1 and 2, X_f will be tangent to the Legendre submanifold $\mathcal{S}$ representing ideal gas, and thus λ_t can be interpreted in each case, at least formally, as a thermodynamic process. In examples 3 and 4, X_f will be transversal to $\mathcal{S}$ and will map (or 'drag') $\mathcal{S}$ for the ideal gas onto $\mathcal{S}$ representing another system. In fact, we will receive a 1-parameter family of new systems.

Let us consider therefore a fluid thermodynamic system having three degrees of freedom. Then its TPS is seven-dimensional. In the energy representation we have the following correspondence:

$$(x^0; p_1, p_2, p_3; x^1, x^2, x^3) \iff (U; -T, P, -\mu; S, V, N), \tag{21}$$

and respectively the contact form is

$$\theta^U \equiv \theta = \mathrm{d}U - T\,\mathrm{d}S + P\,\mathrm{d}V - \mu\,\mathrm{d}N. \tag{22}$$

Let us repeat that unless we restrict ourselves to a three-dimensional Legendre submanifold $\mathcal{S}$ (thermodynamic surface) given by equation $\theta = 0$, all these seven variables are treated as independent.

Example 1. For $f = U - TS + RNT - \mu N$ (R is the standard gas constant), according to (17) we have

$$X_f = U\frac{\partial}{\partial U} + P\frac{\partial}{\partial P} + RT\frac{\partial}{\partial \mu} + (S - RN)\frac{\partial}{\partial S} + N\frac{\partial}{\partial N}, \tag{23}$$

and hence the contact Hamilton equations (19) (defined by the components of X_f) have the form

$$\begin{aligned} &\dot{U} = U, && \dot{T} = 0, && \dot{p} = P, && \dot{\mu} = RT, \\ &\dot{S} = S - RN, && \dot{V} = 0, && \dot{N} = N. \end{aligned} \tag{24}$$

Integral curves of X_f are thus given by

$$\begin{aligned} &U = U_0\,\mathrm{e}^t, && S = (S_0 - RN_0 t)\,\mathrm{e}^t, && V = V_0, && N = N_0\,\mathrm{e}^t, \\ &T = T_0, && P = P_0\,\mathrm{e}^t, && \mu = RT_0 t + \mu_0, \end{aligned} \tag{25}$$

where $U_0, S_0, V_0, \ldots$ denote an initial state. One may note that for an ideal gas $f = 0$ and that X_f is tangent to the Legendre submanifold $\mathcal{S}$ representing this system [8]. Hence equations (25) describe a 'thermodynamic process' with a constant volume V_0 and a constant temperature T_0. It is easy to check that during this 'process' all relations between thermodynamic parameters for ideal gas are preserved, for instance

$$U = \tfrac{3}{2}NRT, \qquad PV = NRT \qquad \text{or} \qquad U = TS - PV + \mu N. \tag{26}$$

The Jacobi matrix $\frac{\partial(U,T,P,\mu,S,V,N)}{\partial(U_0,T_0,P_0,\mu_0,S_0,V_0,N_0)}$ of this transformation induces a linear transformation on fibres of the tangent bundle TM. The determinant of this matrix is equal to $\exp(4t)$.

Example 2. For $f = NRT - \frac{2}{5}TS - \frac{2}{5}\mu N$ one obtains

$$X_f = -\frac{2}{5}T\frac{\partial}{\partial T} + \left(RT - \frac{2}{5}\mu\right)\frac{\partial}{\partial \mu} + \left(\frac{2}{5}S - RN\right)\frac{\partial}{\partial S} + \frac{2}{5}N\frac{\partial}{\partial N}, \tag{27}$$

so

$$\begin{aligned} &\dot{U} = 0, && \dot{T} = -\tfrac{2}{5}T, && \dot{p} = 0, && \dot{\mu} = RT - \tfrac{2}{5}\mu, \\ &\dot{S} = \tfrac{2}{5}S - RN, && \dot{V} = 0, && \dot{N} = \tfrac{2}{5}N. \end{aligned} \tag{28}$$

Integrating these equations we obtain

$$\begin{aligned} &U = U_0, && S = (S_0 - RN_o t)\,\mathrm{e}^{2t/5}, && V = V_0, && N = N_0\,\mathrm{e}^{2t/5}, \\ &T = T_0\,\mathrm{e}^{-2t/5}, && P = P_0, && \mu = (\mu_0 + RT_0 t)\,\mathrm{e}^{-2t/5}. \end{aligned} \tag{29}$$

Again $f = 0$ for the ideal gas and thus equations (29) describe a 'process' with constant volume, pressure and internal energy; the relations (26) are also preserved.

The determinant of the Jacobi matrix is now equal to 1, and the matrix itself is an element of $SL(7, \mathbb{R})$, and even the element of $SL(6, \mathbb{R}) \times 1$.

Example 3. Let us now take two very simple functions $f_1 = bP$ and $f_2 = -aV^{-1}$ where a and b are some non-negative constants. Then $X_{f_1} = b\partial/\partial V$ and $X_{f_2} = (-a/V)\partial/\partial U - (a/V^2)\partial/\partial P$ are not tangent to $\mathcal{S}$ representing an ideal gas, so they cannot be treated as thermodynamic processes. The integral curves of X_{f_1} are such that all coordinates are preserved but the volume V which changes according to $V = V_0 + bt$. Therefore, flow associated with X_{f_1} can be interpreted as a flow dragging $\mathcal{S}$ for our ideal gas into $\mathcal{S}$ representing a gas of non-interacting hard spheres. This means that the deformed $\mathcal{S}$ represents a new system. In fact, we get a 1-parameter family of new Legendre submanifolds $\mathcal{S}_t$ corresponding to the gases of hard spheres. Of course this family contains our original Legendre submanifold $\mathcal{S}$ representing the ideal gas for $t = 0$.

On the other hand, the flow λ_τ corresponding to X_{f_2} is such that it preserves all parameters except U and P which change according to (t has been replaced by a new parameter τ)

$$U = U_0 - \frac{a}{V_0}\tau, \qquad P = P_0 - \frac{a}{V_0^2}\tau. \tag{30}$$

This time one can say that λ_τ maps ideal gas into a gas of interacting point-like particles.

An interesting situation arises if we take $f = f_1 + f_2 = bP - aV^{-1}$. The integral curves of $X_f = X_{f_1} + X_{f_2}$ are such that T, S, N and μ do not change, whereas

$$U = U_0 - \frac{a}{b}\ln\frac{V_0 + bt}{V_0}, \qquad P = P_0 - \frac{at}{V_0(V_0 + bt)}, \qquad V = V_0 + bt. \tag{31}$$

The equation of state for the ideal gas, $P_0V_0 = N_0RT_0$, is no longer preserved and after inserting in it formulae (31) it goes over into an equation of state

$$\left(P + \frac{at}{V(V - bt)}\right)(V - bt) = NRT, \tag{32}$$

which for $t = 1$ resembles the well-known van der Waals equation of state. In fact, for fixed a and b we have obtained a 1-parameter family of van der Waals-like gases.

Example 4. Two other versions of the van der Waals-like gases can be obtained if, instead of one transformation induced by $X_{f_1+f_2}$ of example 3, we consider two consecutive transformations: that of X_{f_1} followed by X_{f_2} and vice versa. We receive two different 2-parameter transformations since the transformations induced by f_1 and f_2 do not commute, i.e. the Lie bracket $[X_{f_1}, X_{f_2}] \neq 0$.

In the first case, when X_{f_1} is followed by X_{f_2}, instead of (32) we receive a 2-parameter family of equations of state

$$\left(P + \frac{a}{V^2}\tau\right)(V - bt) = NRT. \tag{33}$$

The result is different if X_{f_2} is followed by X_{f_1} for which

$$\left(P + \frac{a}{(V - bt)^2}\tau\right)(V - bt) = NRT. \tag{34}$$

As a matter of fact, equation (34) for $t = \tau = 1$ reproduces exactly the standard van der Waals equation.

We hope that it should be possible to find a single function f which would allow us to obtain the van der Waals equation of state from the one for the ideal gas in just one step.

The last example is the standard Legendre transformation.

Example 5 (partial Legendre transformation)**.** Let us consider again a seven-dimensional TPS with local coordinates (3) and go over to new coordinates given by

$$\begin{array}{llll} x^{0'} = x^0 + p_2x^2, & p_{1'} = p_1, & p_{2'} = -x^2, & p_{3'} = p_3, \\ x^{1'} = x^1, & x^{2'} = p_2, & x^{3'} = x^3. & \end{array} \tag{35}$$

This is a partial Legendre transformation which gives transition from the energy representation to the enthalpy representation

$$(U; S, V, N; -T, P, -\mu_1) \quad \Longleftrightarrow \quad (H; S, P, N; -T, -V, -\mu_1). \tag{36}$$

Obviously the enthalpy H is equal to $H = U + PV$, and under this transformation θ^U goes over into the contact form $\theta^H = \mathrm{d}H - T\,\mathrm{d}S - V\,\mathrm{d}P - \mu\,\mathrm{d}N$ connected with the enthalpy representation. The Jacobi matrix of transition (35) has determinant equal to 1, so it is a strict contact transformation.

Of course, we could have taken another Legendre transformation and go over to other representations. However, let us repeat that no Legendre transformation gives transition from the energy to the entropy representation. This can be accomplished only by a more general genuine contact transformation with $\rho = T^{-1} \neq 1$. On the other hand, the entropy S is connected by Legendre transformations with the Massieu functions [1, 2].

4. The structure group of TM^{2n+1}

In the following, the $(n+1)$-dimensional Gibbs space (GS) will be denoted by M^{n+1} while the $(2n+1)$-dimensional TPS will be denoted by M^{2n+1} or (M^{2n+1}, θ).

As mentioned before, the Gibbs space M^{n+1} has no distinguished structure, therefore one can only consider the group of general diffeomorphisms of GS, i.e. the group Diff M^{n+1}. As a result, the structure group of its tangent bundle TM^{n+1} is the general linear group $GL(n+1, \mathbb{R})$ and it is not obvious how it could be reduced to any of its subgroups.

Things look quite different if instead of GS one takes the $(2n + 1)$-dimensional TPS (M^{2n+1}, θ). As it was explained above, TPS has a contact structure and this allows us to reduce the structure group of TM^{2n+1} to subgroups of $GL(2n + 1, \mathbb{R})$.

Before doing this, we shall first recall briefly the notion of transition functions for fibre bundles [15–17].

Let $\{\mathcal{O}_\alpha\}$ be an open covering of M^{2n+1} and let $\pi^{-1}(\mathcal{O}_\alpha) = TM^{2n+1}|_{\mathcal{O}_\alpha}$, where $\pi : TM^{2n+1} \to M^{2n+1}$ stands for the standard projection in the tangent bundle. Let now $\psi_\alpha : \pi^{-1}(\mathcal{O}_\alpha) \to \mathcal{O}_\alpha \times \mathbb{R}^{2n+1}$ be a local trivialization of TM^{2n+1}. Then $\psi_{\alpha\beta} := \psi_\alpha \circ \psi_\beta^{-1}$ is a diffeomorphism of $\mathcal{O}_{\alpha\beta} \times \mathbb{R}^{2n+1}$, where $\mathcal{O}_{\alpha\beta} = \mathcal{O}_\alpha \cap \mathcal{O}_\beta$. Restricted to $x \in \mathcal{O}_{\alpha\beta}$, $\psi_{\alpha\beta}(x)$ is an isomorphism of the typical fibre F of the bundle. Of course, in our case $F = \mathbb{R}^{2n+1}$ and thus all $\psi_{\alpha\beta}$ form the group $GL(2n + 1, \mathbb{R})$. The functions $\psi_{\alpha\beta}$ treated as mappings $\psi_{\alpha\beta} : \mathcal{O}_\alpha \cap \mathcal{O}_\beta \to GL(2n + 1, \mathbb{R})$ are called *transition functions* for TM^{2n+1} with respect to the covering $\{\mathcal{O}_\alpha\}$.

Now, because θ is defined on TPS globally and the volume form $\Omega := \theta \wedge (\mathrm{d}\theta)^n \neq 0$ cannot change sign, M^{2n+1} is orientable [15, 16]. Let us assume that the orientation be positive. Then $GL(2n + 1, \mathbb{R})$ can be reduced to $GL_+(2n + 1, \mathbb{R})$, the group of real $(2n + 1) \times (2n + 1)$ matrices with positive determinant. Moreover, $GL_+(2n + 1, \mathbb{R})$ may be reduced to $SL(2n + 1, \mathbb{R})$, the group of $(2n + 1) \times (2n + 1)$ matrices of determinant one. This last reduction is justified by the fact that in each fibre T_xM we may choose $2n + 1$ linearly independent vectors (a basis) $v_1, \ldots, v_k, \ldots, v_{2n}, v_{2n+1}$ such that

$$\begin{aligned}(\theta \wedge (\mathrm{d}\theta)^n)&(v_1, v_2, \ldots, v_{2n}, v_{2n+1}) \\ &= \sum_\sigma \mathrm{sgn}(\sigma)\theta(v_{\sigma(1)})\,\mathrm{d}\theta(v_{\sigma(2)}, v_{\sigma(3)}) \ldots \mathrm{d}\theta(v_{\sigma(2n)}, v_{\sigma(2n+1)}) = 1,\end{aligned} \tag{37}$$

where the symbol σ denotes permutation of $1, 2, \ldots, 2n, 2n + 1$.

We may go even further because every differential manifold M allows a Riemannian metric [15] and thus we may choose an orthonormal basis and reduce $SL(2n+1, \mathbb{R})$ to $SO(2n+1, \mathbb{R})$.

To this end let us recall that any contact manifold (M^{2n+1}, θ) allows a Riemannian metric [18, 19], and in fact an infinite number of Riemannian metrics which are in a sense compatible with the contact structure. In this paper we shall give two examples of such metrics. Their partial compatibility with the contact structure may be seen e.g. from the term $\theta \otimes \theta$ which they contain (see below), although other reasons also exist [8].

To discuss the problem of metric more thoroughly let us denote for a moment all variables (3) on M^{2n+1} uniformly by y^μ and y^ν, $\mu, \nu = 0, 1, \ldots, 2n$, where

$$y^0 = x^0, \qquad y^i = p_i, \qquad y^{n+i} = x^i, \qquad i = 1, \ldots, n. \tag{38}$$

The metric most frequently used in contact geometry, often called the Sasaki metric, has the form [18, 19]

$$\mathrm{d}l^2 \equiv g_{\mu\nu}\,\mathrm{d}y^\mu\,\mathrm{d}y^\nu = \theta \otimes \theta + \mathrm{d}p_i\,\mathrm{d}p_i + \mathrm{d}x^i\,\mathrm{d}x^i, \tag{39}$$

where $\mathrm{d}y^\mu\,\mathrm{d}y^\nu = (1/2)(\mathrm{d}y^\mu \otimes \mathrm{d}y^\nu + \mathrm{d}y^\nu \otimes \mathrm{d}y^\mu)$. Without the term $\theta \otimes \theta$ the metric would be Euclidean but degenerate. In the contact coordinates (3) it takes the form

$$\mathrm{d}l^2 = \mathrm{d}x^0\,\mathrm{d}x^0 + 2p_k\,\mathrm{d}x^0\,\mathrm{d}x^k + \delta_{ik}\,\mathrm{d}p_i\,\mathrm{d}p_k + (\delta_{ik} + p_i p_k)\,\mathrm{d}x^i\,\mathrm{d}x^k, \tag{40}$$

or in the matrix block form its components are given by

$$(g_{\mu\nu}) = \left(\begin{array}{c|c|c} 1 & 0 & p_1 \cdots p_n \\ \hline 0 & I_n & 0 \\ \hline \begin{matrix} p_1 \\ \vdots \\ p_n \end{matrix} & 0 & \delta_{ik} + p_i p_k \end{array}\right), \tag{41}$$

where I_n denotes an $n \times n$ unit matrix.

This metric has been used by Hernández and Lacomba in a paper entitled *Contact Riemannian Geometry and Thermodynamics* published in 1998 [12]. The metric (39) has nice geometric properties, in particular the vectors $\xi, \mathcal{P}_k, \mathcal{X}_k$ form an orthonormal basis for (M^{2n+1}, θ, g). Thus, $SL(2n+1, \mathbb{R})$ can be reduced to $SO(2n+1, \mathbb{R})$. Unfortunately, thermodynamical meaning of the Sasaki metric is not known, neither on the full TPS nor on the Gibbs space, nor on the Legendre submanifolds $\theta = 0$. Till now no physical applications of this metric are known.

The question how to introduce a metric on the space of thermodynamic variables has been discussed for decades with various intensities. A new impulse in this direction was given after 1975 by a series of five papers by Weinhold [20]. Weinhold's metric tensor was defined only on the n-dimensional surface of thermodynamic states embedded in $(n+1)$-dimensional Gibbs space (in our approach this surface corresponds to a projection of $\mathcal{S}$ from TPS to GS). Components of this metric tensor were given by the second derivatives of the internal energy function. These five papers were followed by dozens of papers discussing the meaning of this metric from various points of view. In particular, many authors discussed the question of metric on the ambient $(n+1)$-dimensional Gibbs space which would reduce to the Weinhold metric.

Another approach to the thermodynamic metric is connected with applications of differential geometry to probability and statistics, and consequently to statistical physics. The notion of *relative entropy* (or relative information) served as a means for introducing a metric in the family of probability distributions. More information and literature on this topic can be found in [8]. Metrics derived from relative entropy have been applied to various thermodynamic systems. The Riemann scalar curvature has been computed and it has been interpreted in terms of fluctuation theory or stability of the considered systems.

The metric based on the concept of relative entropy suggested us a new type of metric on TPS. Using the contact coordinates (3) and the contact form θ this new metric (denoted by capital G) has the form [8]

$$\begin{aligned} dl^2 \equiv G_{\mu\nu}\, dy^\mu\, dy^\nu &= \theta \otimes \theta + dp_i\, dx^i \\ &= dx^0\, dx^0 + 2p_i\, dx^0\, dx^i + dp_i\, dx^i + p_i p_j\, dx^i\, dx^j, \end{aligned} \tag{42}$$

and the matrix of its components is

$$(G_{\mu\nu}) = \left(\begin{array}{c|c|c} 1 & 0 & p_1 \cdots p_n \\ \hline 0 & 0 & \frac{1}{2} I_n \\ \hline p_1 & & \\ \vdots & \frac{1}{2} I_n & p_i p_j \\ p_n & & \end{array}\right). \tag{43}$$

Actually, only the term $dp_i\, dx^i$ was derived in statistical physics from relative entropy. However, there p_i were given by first-order derivatives of a thermodynamic potential, say $p_i = -\partial\phi/\partial x^i$, where the potential ϕ was a function of n independent variables x^k and its physical meaning depended on the probability distribution used; ϕ was proportional to the logarithm of the appropriate partition function.

Thus the term $dp_i\, dx^i$, if applied to an n-dimensional space of thermodynamical states (parametrized by $x^1, \ldots, x^n$), gives the Weinhold metric. So, it could be interpreted thermodynamically in terms of stability conditions. Note that the term $\theta \otimes \theta$ does not contribute if the metric is restricted to the Legendre submanifold $\theta = 0$. It was added only with the purpose of removing degeneracy of the metric $dp_i\, dx^i$ on TPS.

The meaning of the metric (42) on the full TPS and on the Gibbs space is not known yet. Nevertheless, some of its geometrical properties on TPS have been found and will be published in another paper. Let us mention only that the $2n + 1$ vectors $\xi, \mathcal{P}_k, \mathcal{X}_k$ do not form an orthogonal basis for this metric. However, the vector ξ in this metric is in each point orthogonal to the corresponding contact hyperplane spanned by $\mathcal{P}_k$ and $\mathcal{X}_k$. This is sufficient for our purposes because it is possible to construct an orthogonal basis in each contact hyperplane by taking linear combinations of $\mathcal{P}_k$ and $\mathcal{X}_k$.

To continue the reduction procedure let us again turn to the fact that θ defines on M^{2n+1} two complementary distributions, D and Ξ of dimensions $2n$ and 1 respectively, so $SO(2n+1, \mathbb{R})$ can be reduced to $SO(2n, \mathbb{R}) \times SO(1, \mathbb{R}) = SO(2n, \mathbb{R}) \times 1 \cong SO(2n, \mathbb{R})$, where $SO(2n, \mathbb{R})$ acts on D and $SO(1, \mathbb{R})$ on Ξ. In local contact coordinates $d\theta$ is equal to $d\theta = dp_i \wedge dx^i$, therefore the matrix J of its coefficients is equal to

$$J = \frac{1}{2}\begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}. \tag{44}$$

Because $d\theta$ is non-degenerate on D (as a matter of fact $d\theta$ is a symplectic form on D) and $SO(2n, \mathbb{R})$ acts on D, we may restrict ourselves to transition functions (transformations) which do not change $d\theta$, i.e. to $\psi_{\alpha\beta} \equiv H$ commuting with J; $HJ = JH$ or $HJH^T = J$ because for $H \in SO(2n, \mathbb{R})$ the transpose H^T of H is equal to H^{-1}. Thus our group has been additionally reduced to the intersection of the symplectic and orthogonal groups, i.e. to $Sp(2n, \mathbb{R}) \cap O(2n) \times 1$.

However, the commutation condition of J and H requires that H be of the form

$$H = \begin{pmatrix} A & B \\ -B & A \end{pmatrix}, \tag{45}$$

where A and B denote $n \times n$ matrices with real entries. The matrices of type (45) form a subgroup of $GL(2n, \mathbb{R})$; let us denote it by K. Moreover, the subgroup K is isomorphic with the general linear complex group $GL(n, \mathbb{C})$, i.e with the group of non-singular $n \times n$ matrices with complex entries because any matrix Q of $GL(n, \mathbb{C})$ can be written in the form $Q = A + \mathrm{i}B$, where $\mathrm{i} = \sqrt{-1}$ and A and B are real $n \times n$ matrices. The isomorphism $\varphi : GL(n, \mathbb{C}) \to \mathrm{K}$ is then given by the formula

$$\varphi(A + \mathrm{i}B) = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} = H. \tag{46}$$

Our reduced group can be thus written in the form $Sp(2n, \mathbb{R}) \cap GL(n, \mathbb{C}) \times 1$ and also in the form $O(2n, \mathbb{R}) \cap GL(n, \mathbb{C}) \times 1 \equiv U(n) \times 1$. This is the final result of the reduction procedure. The last point can be easily inferred by considering the inverse φ^{-1} of φ for which we have

$$[\varphi^{-1}(H)]^{\dagger} = \overline{\varphi^{-1}(H)}^{T} = \overline{A + \mathrm{i}B}^{T} = (A - \mathrm{i}B)^{T} = \varphi^{-1}(H^{T}) = \varphi^{-1}(H^{-1}) = [\varphi^{-1}(H)]^{-1}. \tag{47}$$

Thus one can see that $\varphi^{-1}(H)$ is a unitary matrix.

The consecutive steps of the whole reduction procedure described above can be therefore summarized in the following diagram:

$$\begin{aligned} GL(2n+1, \mathbb{R}) &\longrightarrow GL_{+}(2n+1, \mathbb{R}) \longrightarrow SL(2n+1, \mathbb{R}) \longrightarrow SO(2n+1, \mathbb{R}) \\ &\longrightarrow SO(2n, \mathbb{R}) \times SO(1, \mathbb{R}) \equiv SO(2n, \mathbb{R}) \times 1 \\ &\longrightarrow Sp(2n, \mathbb{R}) \cap O(2n) \times 1 \longrightarrow GL(n, \mathbb{C}) \cap O(2n) \times 1 \\ &= U(n) \times 1. \end{aligned} \tag{48}$$

Let us remember that the symplectic group has the property [3]

$$Sp(2n, \mathbb{R}) \cap O(2n) = Sp(2n, \mathbb{R}) \cap GL(n, \mathbb{C}) = GL(n, \mathbb{C}) \cap O(2n) = U(n), \tag{49}$$

and this can be recognized in the reduction procedure.

5. Conclusions

We have just shown that for a thermodynamic phase space (M^{2n+1}, θ), the structure group of its tangent bundle can be reduced to $U(n) \times 1$.

Therefore, a manifold M^{2n+1} can be the space of thermodynamic states if its principal bundle can be reduced to the bundle with the group $U(n) \times 1$. This is not possible for an arbitrary $(2n+1)$-dimensional manifold M^{2n+1}. It means that among all $(2n+1)$-dimensional manifolds we may choose only a subclass of such manifolds for which the structure groups of their tangent bundles reduce to $U(n) \times 1$.

The last two formulae of section 4, (48) and (49), contain a lot of information about the symmetries of thermodynamics. They tell us how these symmetries are related e.g. to the symplectic and orthogonal groups. They also tell us, for instance, that—against the common belief—in thermodynamics we are not confined only to Legendre transformations. Section 3 gives a few examples of more general contact transformations.

As a last remark let us stress that although examples of θ were given only for fluid systems, it should be obvious that the whole formalism applies to any thermodynamic system, e.g. to magnetic systems, and to any representation.

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