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A preliminary framework for continuum thermodynamics

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Abstract. We construct a framework for continuum thermodynamics by first defining a setting specifying the states, the observables, the processes, and introducing the energy as a functional on the processes. We then present the postulates; two that add structure to the state manifold (the First and a ‘corollary’ to the Second Law of Thermodynamics) and a third that imposes some conditions on the possible evolutions of an isolated system (the Second Law). As an application, we study the formal relation between the thermodynamic equilibrium states and the thermostatic framework.

1. Introduction

A global approach to the formulation of a physical theory is to give the interrelationship between the set of states, observables, kinematical symmetries and dynamical evolutions. A typical example of such a formulation, is the Abraham–Marsden exposition of classical mechanics [1]. Here the states are represented by the points of a differential manifold M , the observables by functions $0: M \rightarrow \mathbb{R}$, the set of kinematical symmetries that is assumed to form a Lie group, by a regular action of this group on M , and the dynamical action by a piecewise differentiable curve $c: [t_1, t_2] \rightarrow M$. It is assumed that this curve satisfies the equations of motion $\dot{c} = \chi \circ c$, defined by a vectorfield χ on M that expresses the dynamical laws.

In an actual case, a theory can be constructed by starting with a basic structure, the setting, on which further structure is imposed by means of ‘physically’ motivated postulates. The distinction between setting and additional structures is in no way unique, but depends on conventions, taste and convenience. The procedure has the advantage that each of the structures can be studied separately.

The subject of this paper is a construction of continuum thermodynamics. By this we mean a theory for the description of systems characterized by the

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observables of entropy S , momentum Π_i , mass M etc. It is assumed that the states of a system is represented by the points of an infinite dimensional Banach manifold

$$M = \left\{ (s, \pi_i, \rho, \dots) : \mathbb{R}^3 \rightarrow \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}_+ \times \dots \mid \int_{\mathcal{D}} s(x^i) d^3x < \infty, \dots \right\}$$

where $\mathcal{D} \subset X = \mathbb{R}^3$ denote the (fixed) domain occupied by the system. The observables of entropy, momentum and mass are represented by the functions

$$(s, \pi_i, \rho, \dots) \mapsto S(s, \pi_i, \rho, \dots) = \int_{\mathcal{D}} s(x^i) d^3x$$

$$(s, \pi_i, \rho, \dots) \mapsto \Pi_i(s, \pi_i, \rho, \dots) = \int_{\mathcal{D}} \pi_i(x^i) d^3x$$

$$(s, \pi_i, \rho, \dots) \mapsto M(s, \pi_i, \rho, \dots) = \int_{\mathcal{D}} \rho(x^i) d^3x$$

In addition, there exists another observable, the energy⁽²⁾

$$(s, \pi_i, \rho, \dots) \mapsto U(s, \pi_i, \rho, \dots) = \int_{\mathcal{D}} \hat{u}(s(x^i), \pi_i(x^i), \rho(x^i), \dots) d^3x$$

that is a potential or generating function in these variables, i.e. the components of dU are local observables for the system,

$$\hat{T}(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = \partial_s \hat{u}(s(x^i), \pi_i(x^i), \rho(x^i), \dots)$$

$$\hat{v}^i(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = \partial_{\pi_i} \hat{u}(s(x^i), \pi_i(x^i), \rho(x^i), \dots)$$

$$\hat{\mu}(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = \partial_{\rho} \hat{u}(s(x^i), \pi_i(x^i), \rho(x^i), \dots)$$

It is common to refer to these observables, the temperature, the velocity and the chemical potential respectively, as the intensive variables. The entropy, momentum and mass are correspondingly referred to as the extensive variables. These densities also define local observables,

$$\hat{s}(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = s(x^i)$$

$$\hat{\pi}_i(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = \pi_i(x^i)$$

$$\hat{\rho}(s(x^i), \pi_i(x^i), \rho(x^i), \dots) = \rho(x^i)$$

as does the energy density \hat{u} .

In addition to the energy, there always exist two more generating functions, the entropy S in the variables (u, π_i, ρ, \dots) and the Helmholtz free energy F in the variables (T, π_i, ρ, \dots) . Each of the generating functions contains the information about the relations between the local observables. They are related by Legendre transformations.

⁽²⁾ For simplicity we assume for the moment that u does not depend on the gradients of the state variables.

The kinematical symmetry group of this theory is the Galilei group. It will not be discussed in this paper. Neither will the dynamics. Notice however, that the evolution is assumed to be described by a piecewise differentiable curve

$$c: [t_1, t_2] \rightarrow M_u; t \mapsto (s_t(x^i), \pi_{ti}(x^i), \rho_t(x^i))$$

that is a solution of an ordinary differential equation

$$\dot{c} = \chi \circ j_2(c)$$

where $j_2(c)$ denotes the canonical prolongation to second order

$$j_2(c) = (s_t(x^i), \pi_{ti}(x^i), \rho_t(x^i), \dots, \partial_{x^i} s_t(x^i), \dots, \partial_{x^i} \partial_{x^j} \rho_t(x^i), \dots)$$

The notation means that for a system described by generating functions of the form given above, i.e. whose densities do not depend on the gradients of the state variables, the components are local functions of the state variables and their gradients up to second order [2, 3].

This brief account of continuum thermodynamics indicates that we do not have to bother to much about the state manifold M . At least as long as we only restrict ourselves to formal manipulations, it is sufficient to study the densities of the generating functions which themselves are functions on finite dimensional manifolds. Thus, in our ‘example’ above

$$\hat{u}: \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}_+ \times \dots \rightarrow \mathbb{R}; (s, \pi_i, \rho, \dots) \mapsto \hat{u}(s, \pi_i, \rho, \dots)$$

A more elegant and powerful formulation can be given by using the concept of fibred manifold

$$\mathbb{R}^3 \times (\mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}_+ \times \dots) \rightarrow \mathbb{R}^3; (x^i; s, \pi_i, \rho, \dots) \mapsto (x^i)$$

A state is here represented by a section γ ,

$$(x^i) \mapsto \gamma(x^i) = (x^i; s(x^i), \pi_i(x^i), \rho(x^i), \dots).$$

If a model of a system is described by generating functions whose densities are functions of the gradients of the state variables also, we have to consider the jet extension of the fibred manifold. This is a canonical way of accommodating for the extra variables. Thus the canonical coordinates of the first jet extension of our fibre space is noted

$$(x^i; s, \pi_i, \rho, \dots, s_{,j}, \pi_{i,j}, \rho_{,i}, \dots)$$

A section of our original space is canonically prolonged to a section of its first jet extension $j_1(\gamma)$ by

$$a(x^i) \mapsto (x^i; s(x^i), \pi_i(x^i), \rho(x^i), \dots, \partial_{x^j} s(x^i), \dots, \partial_{x^i} \rho(x^i), \dots)$$

Even in this case the formal manipulations can be performed on the finite dimensional manifold by means of operations that imitates the corresponding operations on M ; thus (functional) derivations on M is simulated by the differential operators

$$\nabla_s = \partial_s - \nabla_i \partial_{s,i} + \dots$$

etc., where $\nabla_i = \partial_{x^i} + s_{,i}\partial_s + \pi_{k,i}\partial_{\pi_k} + \rho_{,i}\partial_{\rho} + \dots$ is the total partial derivative with respect to x^i . This works because of the functorial relations between the categories of fibred differential manifolds, its jet extensions, and the Banach manifolds of its sections [4, 5]. The theory of jet extensions provide us with the natural framework for variational calculus and partial differential equations. It supplies the whole arsenal of concepts and methods of differential calculus that is needed in the formulation and study of models of continuum thermodynamics.

We will motivate the ‘axiomatic’ construction of continuum thermodynamics that we are going to expose by discussing the ‘axiomatic’ formulation of the corresponding thermostatic formalism [6]. We will try to indicate how one ideally could reason on the basis of experimental information, to obtain thermostatics.

Assume that we have established that our system can be described by the observables entropy S , volume V , temperature T and pressure p . We study the system by observing how it can be manipulated. A given set of manipulations of the system is described by a curve on $E = \{(S, V, T, p) \in \mathbb{R} \times \mathbb{R}_+^3\}$, and referred to as a process. Whatever manipulations that we do, however, we do not manage to construct processes that passes through any point of E . This means that not all the points of E represent states, i.e. the functions representing the observables S , V , T and p are not independent functions on the states of the system. In fact, we may ‘conclude’ that the set of states form a two dimensional submanifold L of E . In addition to the observables defined above, we can introduce the quantities heat Q and work W . By studying processes in which heat or work is supplied to or subtracted from the system, one may conclude that the amount of heat or work does not only depend on the initial and final states, but also on the kind of manipulations that is being performed. This means that the change of heat ΔQ and change of work ΔW are to be represented as functionals on the processes,

$$\Delta Q(c) = \int_c q$$

$$\Delta W(c) = \int_c w$$

where as part of an operational definition of the observables we may pose

$$q = T dS$$

$$w = -p dV$$

Notice that q and w are one-forms on E .

Manipulating the system we get the impression that it is sufficient to keep track of the volume and the temperature which also are the most easily controllable observables. We can not know *a priori* if $\{(V, T)\}$ gives a complete parametrization of the states of the system (L might fold over $\{(V, T)\}$); however, we still define a process to be cyclic (or closed) whenever it ends at a state with the same volume and temperature as it started. With this definition at hand we may draw a further conclusion from our manipulations on the system. It turns out that the variation of energy $\Delta E = \Delta Q + \Delta W$ along any cyclic process is zero. Since any process described by a closed curve on L is a cyclic process, this means that the restriction of the one-form $\theta_U = T dS - p dV$ to L is closed, i.e. L is a Lagrangian

submanifold of the symplectic manifold $(E, d\theta_U)$. On the other hand, if L folds over $\{(V, T)\}$, then there exists cyclic processes described by curves that are not closed on L . Since $\Delta E(c)$ could not be zero on all such cyclic processes, we must conclude that such processes can not exist, i.e. L can not fold over $\{(V, T)\}$. In other words, $\{(V, T)\}$ gives a complete parametrization of the states. From the theory of Lagrangian manifolds it then also follows that L is globally described by the generating function $F: \{(V, T)\} \rightarrow \mathbb{R}$, the Helmholtz free energy, i.e.

$$p(V, T) = -\partial_V F(V, T)$$

$$S(V, T) = -\partial_T F(V, T)$$

The next assumption we make is that $\partial_T^2 F < 0$. In the context of continuum thermodynamics this is a stability condition; it is not equivalent to, but a 'corollary' to the Second Law of thermodynamics (see paragraph 4). The condition expresses in some sense the non-dynamical content of the Second Law.

$-\partial_T^2 F$ is the Jacobian determinant of the map

$$\{(V, T)\} \rightarrow \{(S, V)\}; (V, T) \mapsto (-\partial_T F(V, T), V)$$

and the stability condition ensures therefore the existence of the energy function as a global generating function. Since $T = \partial_S U$ is the Jacobian of the map

$$\{(S, V)\} \rightarrow \{(U, V)\}; (S, V) \mapsto (U(S, V), V)$$

the positivity of the temperature implies the existence of the entropy as a global generating function.

We have thus outlined a possible construction of the framework of thermostatics [6]. The framework for continuum thermodynamics exposed in this paper is quite analogous, and one could imagine to justify it by similar arguments. It is more natural however, to consider the problem to be that of constructing the thermodynamical framework in such a way that *a posteriori* the structure on the set of equilibrium states (thermostatic states) is inherited from the analogue structure on the thermodynamical state space.

The equilibrium states of a thermodynamical system are by definition the states that maximize the entropy with respect to a set of variations that leaves invariant the set of conserved quantities: energy, momentum, mass and angular momentum. According to the 'Second Law of Thermodynamics', these are also the asymptotic states for the evolution of the isolated system. It is (mathematically) inconceivable that the structure on the thermostatic states (Lagrangian submanifold and generating functions) can be obtained from thermodynamics by a maximizing process if it is not already present on that level. This is the methodological justification for our construction.

Our formulation of thermostatics and thermodynamics differs from most others in two respects; by the explicit introduction and use of the concept of Lagrangian submanifold, and by a different use of the 'Laws of Thermodynamics'. The theory of Lagrangian submanifolds gives the global geometrical setting for the definition of generating functions and Legendre transformations. An immediate consequence of this geometrization of the language of thermodynamics is that we can extract more information from the 'Laws of Thermodynamics'. In particular the First Law implies not only that the Helmholtz free

energy is represented as a function on the states, but also that a given set of variables gives a complete parametrization of the states, the set of variables in which the Helmholtz free energy is a generating function. Moreover, from other postulates one ensures the global existence of the energy and the entropy as generating functions. Other naturally definable generating functions like the Gibbs free energy and the enthalpy has only a local existence. The reason for this is that the corresponding set of variables does not necessarily give a complete parametrization of the states: the canonical projection of the state manifold L onto the submanifold defined by these variables might be singular. When this is the case the system is said to possess phase transitions and it means that the classification of phases and methods for the study of the behavior of a system in a state close to a singularity or the construction of the equilibrium states is supplied by the theory of Lagrangian singularities [7].

A main motivation for the research summarized in this paper has been to understand how to describe and classify the different kinds of ‘phase-transitions’. In order to do that one must *a priori* consider a theory like continuum thermodynamics, that is more general than thermostatics, and then study the conditions that define the equilibrium states. The equilibrium conditions for a thermodynamic system consist of extremal conditions and stability or maximum conditions. Except for a class of conditions derived by means of variations due to local variations of volume, there are two kinds of extremal conditions. One kind appears from the variations in the ‘direction’ of the conserved quantities. The resulting conditions tell that the gradients of the corresponding intensive observables are zero on the equilibrium states. These conditions gives rise to the parameters used to parametrize the thermostatic states. Moreover, the existence of phase-transitions of the first kind depends on the properties of these conditions. The other kind appears from the variations in the ‘directions’ of the non-conserved quantities, often referred to as the order-parameters. These conditions simply tell that the corresponding intensive observables are zero on the equilibrium states. There is thus no direct trace of the order parameters in thermostatics, however, the possible existence of phase-transitions of the second class is determined by these conditions.

Part I: The Framework of Thermodynamics

2. The setting

We will start by introducing some spaces. We will denote by $\mathcal{E} \rightarrow X$, $\mathcal{E}_s \rightarrow X$ and $\mathcal{E}_T \rightarrow X$ the fibred manifolds, where

$$\mathcal{E} = \{(x^i; \pi_i, \rho, \eta_\alpha, \phi^\alpha) \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}_+ \times \mathcal{M}\}$$

$$\mathcal{E}_s = \{(x^i; s) \in \mathbb{R}^3 \times \mathbb{R}\}$$

$$\mathcal{E}_T = \{(x^i; T) \in \mathbb{R}^3 \times \mathbb{R}\}$$

\mathcal{M} is here assumed to be a $2n$ -dimensional manifold and η_α, ϕ^α are coordinates on M . We will use the symbol \oplus to denote the fibred or Whitney product; thus, for example,

$$\mathcal{E}_s \oplus \mathcal{E}_T = \{(x^i; s, T) \in \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}_+\}$$

Definition. A thermodynamic system is by assumption associated with⁽³⁾

- i) a statemanifold that is a differentiable Banach manifold \mathcal{B} of sections $X \rightarrow I$, where

$$\begin{aligned} I &\subset \mathcal{E}_s \oplus \mathcal{E}_T \otimes V_r^* J_{2q}(\mathcal{E}) \\ &= \{(x^i; s, T, \pi_i, \rho, \eta_\alpha, \phi^\alpha, \pi_{i,j}, \rho_{,j}, \eta_{\alpha,j}, \phi_{,j}^\alpha, \dots, v^i, \mu, v^\alpha, \kappa_\alpha) \varepsilon \dots\} \end{aligned}$$

- ii) the *extensive* ‘observables’ entropy density s , momentum density π_i , mass density ρ and internal (extensive) observables η_α, ϕ^α , and the *intensive* observables temperature T , velocity v^i , chemical potential μ and internal intensive observables v^α and κ_α are represented by the restriction of the functions $\mathcal{E}_s \oplus \mathcal{E}_T \oplus V_r^* J_{2q}(\mathcal{E}) \rightarrow \mathbb{R}$

$$\begin{aligned} \hat{s}(x^i; s, \dots) &= s \\ &\vdots \\ \hat{\kappa}_\alpha(x^i; s, \dots) &= \kappa_\alpha \end{aligned}$$

to I ;

- iii) a set of processes, i.e. sectionvalued ‘curves’

$$c: X \times [t_1, t_2] \rightarrow \mathcal{E}_s \oplus \mathcal{E}_T \oplus \mathcal{E}$$

such that its prolongation $\bar{c}_t \varepsilon I \forall t \in [t_1, t_2]$.

- iv) a quantity called energy whose variation ΔE along a process c is measured by the 1-form

$$\theta_u = T ds + v^i d\pi_i + \mu d\rho + v^\alpha d\eta_\alpha + \kappa_\alpha d\phi^\alpha$$

i.e.

$$\Delta E(c) = \int_c \theta_u = \int_{[t_1, t_2] \times \mathbb{R}^3} \theta_u(\dot{c}) \circ c d^3x dt$$

3. The First Law of Thermodynamics

Definition. Let π_f denote the projection (submersion)

$$\mathcal{E}_s \oplus \mathcal{E}_T \oplus V_r^* J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_T \oplus J_{2q}(\mathcal{E})$$

⁽³⁾ For the notation, see the appendix.

a process is said to be closed if its prolongation \tilde{c} is closed, i.e.

$$\pi_f \circ \tilde{c}: [t_1, t_2] \rightarrow \mathcal{E}_T \oplus J_{2q}(\mathcal{E})$$

is closed; $\pi_f \circ \tilde{c}(t_1) = \pi_f \circ \tilde{c}(t_2)$.

Postulate 1D: (The First Law of Thermodynamics):

a) the variation of energy is zero along any closed process c , i.e.

$$\Delta E(c) = 0$$

b) $\pi_f | l: l \rightarrow \mathcal{E}_T \oplus J_{2q}(\mathcal{E})$ is surjective.

An equivalent statement is expressed by the following theorem which we will refer to as the *First Fundamental Theorem of Thermodynamics*.

Theorem. *Postulate 1D is equivalent to the following statements:*

- i) l is a ‘Lagrangian’ submanifold of $(\mathcal{E}_s \oplus \mathcal{E}_T \oplus V_r^* J_{2q}(\mathcal{E}), d\theta_u)^{(4)}$
- ii) $\pi_f | l: l \rightarrow \mathcal{E}_T \oplus J_{2q}(\mathcal{E})$ is nonsingular.

Proof. Modulo some manipulations discussed in the appendix, the proof follows that of the corresponding thermostatic theorem [6]. ■

Corollary. *There exists a global generating function (density) $f: \mathcal{E}_T \oplus J_{2q}(\mathcal{E}) \rightarrow \mathbb{R}$, the Helmholtz free energy-density, i.e. there exists a Lagrangian submersion $\phi_f: \mathcal{E}_T \oplus J_{2q}(\mathcal{E}) \rightarrow l$ such that $\phi_f(\mathcal{E}_T \oplus J_{2q}(\mathcal{E})) = l$ and $\phi_f^* \theta_f = df$ for $\theta_f = \theta_u - d(sT)$.⁽⁵⁾*

Proof. The proof follows closely the proof of the corresponding corollary in Paragraph 3 [6]. See also the appendix. Notice that

$$\phi_f: \mathcal{E}_T \oplus J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_s \oplus \mathcal{E}_T + V_r^* J_{2q}(\mathcal{E})$$

$$(x^i; T, \pi_i, \dots) \mapsto$$

$$(x^i; -\partial_T f(x^i; T, \dots), T, \pi_i, \dots, \nabla_{\pi_i} f(\cdot), \nabla_{\rho} f(\cdot), \nabla_{\eta_\alpha} f(\cdot), \nabla_{\phi^\alpha} f(\cdot)) \quad \blacksquare$$

The above theorem assures the existence of a representation, the free energy representation.⁽⁶⁾

Definition. In the free energy representation

- i) the statemanifold $\mathcal{B}(\mathcal{E}_T \oplus \mathcal{E})$ is a Banach-manifold of sections of $\mathcal{E}_T \oplus \mathcal{E} \rightarrow X$

⁽⁴⁾ In the generalized sense defined in the appendix.

⁽⁵⁾ It is defined modulo a divergence term $\nabla_i g^i(\cdot)$.

⁽⁶⁾ The preceding exposition of the framework of thermodynamics is unfortunately a bit too sketchy. Any attempt of mathematical completeness would however, demand too much space.

ii) the observables are represented by function $\mathcal{E}_T \oplus J_{2q}(\mathcal{E}) \rightarrow \mathbb{R}$ defined by

$$\begin{aligned} s_f(x^i; T, \dots) &= -\partial_T f(x^i; T, \dots) \\ T_f(x^i; T, \dots) &= T \\ &\vdots \\ \kappa_{f\alpha}(x^i; T, \dots) &= \nabla_{\phi^\alpha} f(x^i; T, \dots). \end{aligned}$$

4. The energy and entropy representations

The First Law of Thermodynamics assures the existence of the free energy representation. To get further, we must introduce other postulates. In particular, the considerations in [6] suggest that if we assume that $\partial_{Tf}^2 \hat{f} < 0$, then we can derive the existence of the energy and entropy representations. The Second Law of Thermodynamics tells that an isolated system evolves towards a state, an equilibrium state, and that this is a state that maximizes the entropy function with respect to variations that leave invariant the energy, the momentum and the mass. The equilibrium states thus satisfy two kinds of conditions, the extremal conditions which are first order differential conditions, and the maximum conditions which are second order differential conditions. These maximum conditions are expressed by the matrix of second derivatives of the entropy. It should be negative definite on the equilibrium states. Transformed to the free energy representation this matrix changes sign and decomposes into two blocks. One block is simply $\partial_{Tf}^2 \hat{f}$, which thus should be negative on the equilibrium states. Accordingly, somehow the condition $\partial_{Tf}^2 \hat{f} < 0$ is a ‘corollary’ of the Second Law. This argument is however circular. If we assume *a priori* that $\partial_{Tf}^2 \hat{f} < 0$, then we can derive the existence of the entropy representation and prove from the Second Law that $\partial_{Tf}^2 \hat{f} < 0$. If we do *not* assume that $\partial_{Tf}^2 \hat{f} < 0$, then we can *not* derive the existence of the entropy representation and we can *not* prove from the Second Law that $\partial_{Tf}^2 \hat{f} < 0$.

Postulate 2D: The free energy density f satisfies the stability condition

$$\partial_{Tf}^2 f < 0.$$

Theorem. The map ϕ_{fu} defined by

$$\mathcal{E}_T \oplus J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_s \oplus J_{2q}(\mathcal{E}); (x^i; t, \pi_i, \dots) \mapsto (x^i; -\partial_T f(\cdot), \pi_i, \dots)$$

is a diffeomorphism.

Proof. The Jacobian matrix of ϕ_{fu} is $-\partial_{Tf}^2 \hat{f} \neq 0$. ■

Corollary. There exists a generating function $\hat{u}: \mathcal{E}_s \oplus J_q(\mathcal{E}) \rightarrow \mathbb{R}$, the energy-density, i.e.

$$\exists \phi_u: \mathcal{E}_s \oplus J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_s \oplus \mathcal{E}_T \oplus V_r^* J_{2q}(\mathcal{E})$$

such that

$$\phi_u(\mathcal{E}_s \oplus J_{2q}(\mathcal{E})) = l \ \& \ \phi_u^* \theta_u = d\hat{u}$$

The proof of this and the following statements are essentially the same as the corresponding theorems in [6].

Theorem. Let ϕ_{uf} denote the inverse of ϕ_{fu} ; then,

$$\hat{u} = \hat{f} \circ \phi_{uf} - s\hat{T} \circ \phi_{uf}$$

Theorem. The map ϕ defined by

$$\begin{aligned} \mathcal{E}_s \oplus \mathcal{E}_T \oplus V_r^* J_{2q}(\mathcal{E}) &\rightarrow \mathcal{E}_u \oplus \mathcal{E}_{1/T} \oplus V_r^* J_{2q}(\mathcal{E}) \\ (x^i; s, T, \pi_i, \dots) &\mapsto \left(\hat{u}(\cdot), \frac{1}{T}, \pi_i, \dots \right) \end{aligned}$$

is a diffeomorphism; moreover, the projection of l into $\mathcal{E}_u \oplus J_{2q}(\mathcal{E})$ is a submersion.

Corollary. There exists a generating function $\hat{s}: \mathcal{E}_u \oplus J_{2q}(\mathcal{E}) \rightarrow \mathbb{R}$, the entropy, i.e.

$$\phi_s: \mathcal{E}_u \oplus J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_u \oplus \mathcal{E}_{1/T} \oplus V_r^* J_{2q}(\mathcal{E})$$

such that

$$\phi_s(\mathcal{E}_u \oplus J_{2q}(\mathcal{E})) = l \ \& \ \phi_s^* \theta_s = d\hat{s}$$

where

$$\theta_s = \frac{1}{T} du - \frac{v^i}{T} d\pi_i - \frac{\mu}{T} d\rho - \frac{v^\alpha}{T} d\eta_\alpha - \frac{\kappa_\alpha}{T} d\phi^\alpha$$

The Second Law and the dynamics

The evolution of a thermodynamic system during a time interval $[t_1, t_2]$ is described by a curve c on the state manifold $\mathcal{B}(\mathcal{E}_s \oplus \mathcal{E})$. c is a generalized solution of an ordinary differential equation in $\mathcal{B}(\mathcal{E}_s \oplus \mathcal{E})$. The equation of motion

$$\dot{c} = \chi \circ j_q(c)$$

where denote the symbol for the dynamical vectorfield on $\mathcal{B}(\mathcal{E}_s \oplus \mathcal{E})$. $\chi = \chi^\alpha \nabla_{y^\alpha}$ is represented as a differential operator on $\mathcal{E}_s \oplus J_q(\mathcal{E})$, its coefficients are functions on $J_2(\mathcal{E}_s) \oplus J_{q+2}(\mathcal{E})$. The only explicit assumption usually given is the following version of the Second Law of Thermodynamics (Clausius–Duhem):

The evolution c of an isolated system satisfy

$$\int_{c(t_2)} s d^3x \geq \int_{c(t_1)} s d^3x, \quad \forall t_2 > t_1.$$

We will however make some further assumptions, and refer to the following postulate as the Dynamical Postulate:

Postulate 3D: The dynamics of an isolated system is supposed to be described by a vectorfield χ such that

$$\text{a) } \chi = \chi^H + \chi^G$$

with

$$\chi^H(s) = \nabla_i \xi_s^{Hi} \ \& \ \int_{\gamma} \chi^G(s) d^3x \geq 0, \quad \forall \gamma \in \mathcal{B}(\mathcal{E})$$

$$\text{(b) } 1) \ \chi^H(u) = \nabla_i \xi_u^{Hi} \ \& \ \chi^G(u) = \nabla_i \xi_u^{Gi}$$

$$2) \ \chi^H(\pi_i) = \nabla_j \xi_{\pi_i}^{Hj} \ \& \ \chi^G(\pi_i) = \nabla_j \xi_{\pi_i}^{Gj}$$

$$3) \ \chi^H(\rho) = \nabla_i \xi_{\rho}^{Hi} \ \& \ \chi^G(\rho) = \nabla_i \xi_{\rho}^{Gi}$$

$$4) \ \chi^H(l_i) = \nabla_m (\varepsilon_{ijk} \delta^{kl} x^j \xi_{\pi_l}^{Hm}) \ \& \ \chi^G(l_i) = \nabla_m (\varepsilon_{ijk} \delta^{kl} x^j \xi_{\pi_l}^{Gm})$$

The conditions under a) express that the dynamical vectorfield can be given as the sum of two terms, one that conserves the total entropy, and one with respect to which the total entropy is a Lyapounov function. The conditions under b) moreover, tells that each of the two terms conserves the energy (1), the total momentum (2), the total mass (3) and the total angular momentum (4).

The dynamical postulate does not give any information about the functional form of the components of the symbol χ (or symbols χ^H and χ^G). This form is most usually established on the basis of considerations evoking the interpretation (and definition) of the basic quantities and the 'physical laws' like for example Newton's laws [8]. The results of such considerations must *a posteriori* satisfy the requirements of the dynamical postulate.

In two recent papers [2, 3] we have shown that similar results can be obtained by assuming that χ^H is a Hamiltonian vectorfield: 'There exist symplectic structures such that the Hamiltonian vectorfield with the energy \hat{u} as Hamiltonian satisfies the dynamical postulate'. While the more traditional way of establishing χ^H becomes impracticable for systems with several chemical components, the Hamiltonian method has the advantage that it applies as easily to N -component systems as 1-component systems.

This last remark also applies to our construction of χ^G . We assume that χ^G is a gradient field constructed from a family of functions of the form $\tilde{r} = r \circ \psi$. In the examples we have considered, \tilde{r} is essentially a function of rotation invariant combinations of the (extremal) equilibrium conditions. The gradient is computed with respect to the intensive variables in the entropy representation and the result turned into a vectorfield by an Euclidean metric with the signatures of the entropy 1-form.

According to this theory, the complete information about a system is thus contained in two functions u and r and a map. This means that the task of constructing and testing models by successive trial and error, is much simplified. This concerns in particular the tests of the behaviour at the equilibrium, the

information about which is entirely contained in the energy function, the free energy function, or the entropy function.

Part II: The Topology of the Thermostatistics statemanifold

6. The equilibrium conditions and the equilibrium map

The Second Law of Thermodynamics tells us that the entropy is monotonically increasing during the evolution of an *isolated* system, i.e. a system that is shielded from outside influence. Energy, momentum and mass are then constants of motion. The possible final states, being point attractors for the evolution, are called equilibrium states. They form a submanifold of the statemanifold of the system, and can be determined as the maxima of the entropy with respect to the class of variations that leaves invariant energy, momentum, angular momentum and mass, and contains the local deformations. The thermostatic statemanifold furnishes a parametrization of the equilibrium states, expressed as a map from the thermostatic statemanifold into the thermodynamic statemanifold. By the pull-back of the 'equilibrium map' the topological structure of the equilibrium statemanifold is imposed on the thermostatic statemanifold (or on the thermostatic potential functions).

The equilibrium map is determined by the maximum conditions on the entropy. To see how this happens we will derive these conditions. The first step is to express the class of variations. These are the variations $\tau = \{\chi\}$ generated by the local deformations of the system, which are expressed by the vectorfield on statespace [4],

$$(\nabla_i(u\xi^i), \pi_j\nabla_i\xi^j + \nabla_i(\pi_j\xi^i), \nabla_i(\rho\xi^i), \dots)^{(7)}$$

where ξ^i is a vectorfield on X tangent to the boundary ∂ of the domain $\mathcal{D} \subset X$ containing the fluid; and by the vectorfields on the state space with components of the form

$$\begin{aligned} \chi(\hat{u}) &= \nabla_i \xi_u \\ \chi(\hat{\pi}_i) &= \nabla_k \xi_{\pi_i}^k + \delta_{ij} \delta^{jl} \nabla_j \xi_{\pi_l}^k \\ \chi(\hat{\rho}) &= \nabla_i \xi_\rho^i, \quad \chi(\hat{\eta}_\alpha) = \chi_{\eta_\alpha}, \quad \chi(\hat{\phi}^\alpha) = \chi_{\phi^\alpha} \end{aligned}$$

The extremal conditions then read

$$\chi(s) = 0 \quad \forall \chi \in \tau$$

⁽⁷⁾ To specify the η_α and ϕ^α components we must know how the group $GI(3)$ acts in \mathcal{M} .

or in more detail; the variations induced by local deformations give

$$\nabla_j \left\{ \frac{1}{T} (\pi_i v^j + P_i^j - \delta_i^j (-u + sT + \pi_k v^k + \rho\mu)) + \dots = 0 \right. \quad (8)$$

where $P = P_\pi + P_\rho$ is non-zero if u depends on the gradients of π or ρ . The general expression for P is given in Paragraph 4 [2]. The variations in the other directions give

$$\begin{aligned} \nabla_i \partial_u \hat{s} &= 0 \\ \nabla_i \nabla_{\pi_j} \hat{s} + \delta_{ik} \delta^{jl} \nabla_l \nabla_{\pi_k} \hat{s} &= 0 \\ \nabla_i \nabla_\rho \hat{s} &= 0 \\ \nabla_{\eta_\alpha} \hat{s} &= 0 \ \& \ \nabla_{\phi^\alpha} \hat{s} = 0 \end{aligned}$$

or equivalently⁽⁹⁾

$$\begin{aligned} \partial_u \hat{s} &= \frac{1}{T} = \text{const.} \\ \nabla_{\pi_i} \hat{s} &= \frac{1}{T} v^i = \text{const.} \\ \nabla_\rho \hat{s} &= \frac{1}{T} = \text{const.} \\ \nabla_{\eta_\alpha} \hat{s} &= 0 \ \& \ \nabla_{\phi^\alpha} \hat{s} = 0 \end{aligned}$$

The stability or maximum condition is expressed by

Hess $s =$ (matrix of second derivatives of \hat{s})

is negative definite on the maxima, These conditions can also be expressed in the free energy representation.

Theorem. *In the free energy representation the equilibrium conditions read*

i) *the extremal conditions*

$$\begin{aligned} \nabla_j (\pi_i v^j + P_i^j + \delta_i^j (-f_T + \pi_k v^k + \rho\mu)) &= 0 \\ \nabla_{\pi_i} f_T(\dots) &= v^i \\ \nabla_\rho f_T(\dots) &= \mu \\ \nabla_{\eta_\alpha} f_T(\dots) &= 0 \\ \nabla_{\phi^\alpha} f_T(\dots) &= 0 \end{aligned}$$

where the $f_T(\dots) = f(T, \dots)$ and $(T, v^i, \mu) \in \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}$;

ii) *the stability conditions*

Hess $f_T =$ (matrix of second derivatives of the family of functions f_T)
is positive definite.

⁽⁸⁾ The nonspecified term is a function of $\eta_\alpha, \phi^\alpha, \nabla_{\eta_\alpha} \hat{u}, \nabla_{\phi^\alpha} \hat{u}$ and their derivatives. It will in view of the other extremal conditions be zero.

⁽⁹⁾ We assume $v^i = 0$ on $\partial \mathcal{D}$.

Proof

- i) is obtained by a simple transcription from one representation to the other.
 ii) follows from a standard transformation of the Hessian matrix by the Jacobi matrix of the diffeomorphism

$$\phi_{sf}: \mathcal{E}_u \oplus J_{2q}(\mathcal{E}) \rightarrow \mathcal{E}_T \oplus J_{2q}(\mathcal{E})$$

i.e. by the formula

$$A_{ij}(x^i) \mapsto A_{ij}(\phi^i(y^i)) \partial_{y^k} \phi^i(y^i) \partial_{y^l} \phi^j(y^j)$$

As a result one gets

$$\text{Hess}(\hat{s}) \mapsto -\frac{1}{T} \begin{bmatrix} -\partial_T^2 f & 0 \\ 0 & \text{Hess}(f_T) \end{bmatrix} \blacksquare$$

The solution to the equilibrium conditions are thus *a priori* parametrized by the intensive thermostatic variables⁽¹⁰⁾

$$(T, \mu) \mapsto (s_{(T,\mu)}(x), \pi_{(T,\mu)i}(x), \dots)$$

i.e. the solutions define a map from the space of the intensive thermostatic variables to the thermodynamic statemanifold. However, by combining the map defined by

$$(s(x), \rho(x), \eta_\alpha(x), \phi^\alpha(x)) \mapsto \left(\frac{1}{V} \int_{\mathcal{Q}} s(x) d^3x, \frac{1}{V} \int_{\mathcal{Q}} \rho(x) d^3x \right)$$

from the thermodynamic statemanifold onto the space of extensive thermostatic density variables, with the injection of the equilibrium statemanifold into the thermodynamic statemanifold, we can construct a parametrization of the equilibrium states by these variables, i.e.

$$(s, \rho) \mapsto (s_{(s,\rho)}(x), \rho_{(s,\rho)}(x), \eta_{\alpha(s,\rho)}(x), \phi_{(s,\rho)}^\alpha(x))$$

where

$$\frac{1}{V} \int_{\mathcal{Q}} s_{(s,\rho)}(x) d^3x = s \quad \& \quad \frac{1}{V} \int_{\mathcal{Q}} \rho_{(s,\rho)}(x) d^3x = \rho$$

This is necessary when the system possesses phase-transitions of the first kind. In fact, then a parametrization by the intensive variables (except T) leads to a singular behaviour at the phase transition, indicating a non-uniqueness in this parametrization of the equilibrium states. A simple model on which this phenomenon can be studied is the van der Waal fluid that has been discussed in [6].

⁽¹⁰⁾ We chose $v^i = 0$ and $\pi_i = 0$, i.e. we assume that we consider the solution in the center of mass frame of reference.

Let ϕ denote the map

$$E' \rightarrow \mathcal{B}(\mathcal{E}_T \oplus \mathcal{E}_s) \oplus T^*\mathcal{B}(\mathcal{E})$$

$$(s, \rho, T, \mu) \mapsto (T, s_{(s,\rho)}(x), \rho_{(s,\rho)}(x), \eta_{\alpha(s,\rho)}(x), \phi_{(s,\rho)}^\alpha(x), \mu, 0_\alpha, 0^\alpha)$$

The energy 1-form of thermostatics can then be seen to be the pullback by ϕ of the energy 1-form of thermodynamics;

$$\begin{aligned} \phi^* \int (T(x) ds(x) + \mu(x) d\rho(x) + v^\alpha(x) d\eta_\alpha(x) + \kappa_\alpha(x) d\phi^\alpha(x)) d^3x \\ = T \int_{\mathcal{D}} ds_{(s,\rho)}(x) d^3x + \mu \int_{\mathcal{D}} d\rho_{(s,\rho)}(x) d^3x = (T ds + \mu d\rho)V \end{aligned}$$

Moreover, the thermostatic statemanifold $L' \subset E'$ is the pullback under ϕ of the equilibrium statemanifold $Eql \subset l$. It is evident that L' is a Lagrangian submanifold since l is, and ϕ is a symplectic map. In other words, the postulates of thermodynamics becomes corollaries of the postulates of thermodynamics via this construction.

From now on we will exclusively speak about *classical fluids*, meaning by that fluids described by energy function densities that depends only on the extensive density variables, and not their gradients. One of the remarks made above is then reformulated in the following definition.

Definition. A classical fluid is said to possess phase transitions of the first kind if the projection of l onto $\mathcal{E}_T \oplus \mathcal{F}'$, with $\mathcal{F}' = \{(x^i; \mu, \eta_\alpha, \phi^\alpha) | \dots\}$ is singular.

Thus, if a classical fluid does not possess phase transitions of the first kind, the change of variables

$$\mathcal{E}_u \oplus \mathcal{E} \rightarrow \mathcal{E}_T \oplus \mathcal{F}' : (u, \rho, \eta_\alpha, \phi^\alpha) \mapsto (T, \mu, \eta_\alpha, \phi^\alpha)$$

is a diffeomorphism. There then exists a further representation, the *work representation*.

Theorem. In the work representation the equilibrium conditions read

i) *the extremal conditions*

$$\begin{aligned} p_{(T,\mu)}(\eta_\alpha(x), \phi^\alpha(x)) &= p \\ \partial_{\eta_\alpha} p_{(T,\mu)}(\eta_\alpha(x), \phi^\alpha(x)) &= 0 \\ \partial_{\phi^\alpha} p_{(T,\mu)}(\eta_\alpha(x), \phi^\alpha(x)) &= 0 \end{aligned}$$

ii) *the stability condition*

$$\text{Hess}(p_{(T,\mu)}(\dots)) > 0$$

Proof. This results follows partly from the fact that p denotes the density of the generating function A in the variables $(T, \mu, \eta_\alpha, \phi^\alpha)$. It is obtained by a Legendre transformation from either the energy or the free energy, i.e. as we

have seen in the preceding section, numerically,

$$\begin{aligned} p &= -u + Ts + \mu\rho + v^\alpha\eta_\alpha + \kappa_\alpha\phi^\alpha \\ &= -f + \mu\rho + v^\alpha\eta_\alpha + \kappa_\alpha\phi^\alpha \end{aligned}$$

Moreover, one shows easily that

$$\text{Hess}(s) \mapsto -\frac{1}{T} \begin{bmatrix} \text{Hess}(p_{(T,\mu)}(\cdot, \cdot)) & & 0 \\ 0 & -\partial_T^2 p & -\partial_T \partial_\mu p \\ & -\partial_T \partial_\mu p & -\partial_\mu^2 p \end{bmatrix}$$

which proves the stability conditions. ■

Again the original stability conditions decomposes. We get a condition $\text{Hess } p_{T\mu}$ positive definite, which is a condition on the equilibrium states, and thus a stability condition, and we get the condition that

$$\begin{bmatrix} \partial_T^2 p & \partial_T \partial_\mu p \\ \partial_T \partial_\mu p & \partial_\mu^2 p \end{bmatrix}$$

is negative definite, which expresses a condition on the generating function p and thus on the constitutive relations for systems that do not possess phase transitions of the first kind. Clearly, this condition should be expressed as a postulate for these systems.

7. Phase transitions of the second kind

Assume that we consider a model of a thermodynamic system that does not possess phase transitions of the first kind. As we have seen in Paragraph 6, the equilibrium states of the system minimize the family of functions $A_{T\mu}$ defined by

$$A_{T\mu}: (\eta_\alpha(x), \phi^\alpha(x)) \mapsto \int_{\mathcal{D}} p_{T\mu}(\eta_\alpha(x), \phi^\alpha(x)) d^3x$$

In the great majority of models found in the literature on the subject, the states and the generating functions are subjected to the covariance requirement under a given action of a given group G being the direct product of a group describing the symmetries of space⁽¹¹⁾ and a group describing the internal symmetries of the system. The action of G on \mathcal{M} is induced by equivariant actions σ and Σ on \mathcal{D} and \mathcal{M} , i.e. such that

$$\begin{array}{ccc} \mathcal{D} & \xrightarrow{(\eta_\alpha, \phi^\alpha)} & \mathcal{M} \\ \sigma_\kappa \downarrow & & \downarrow \Sigma_\kappa \\ \mathcal{D} & \xrightarrow{(\eta_\alpha, \phi^\alpha)} & \mathcal{M} \end{array}$$

⁽¹¹⁾ In a complete exposition of thermodynamics one would also speak about the time dependent relativity transformations.

One should notice that $\sigma_g = id$ for all g that describe pure internal symmetries and that σ leaves invariant the Lebesgue measure on \mathcal{D} . Thus, the subgroup H of G that leaves invariant $A_{T\mu}$ satisfy

$$\sigma_g(\mathcal{D}) = \mathcal{D} \ \& \ p_{T\mu} \circ \Sigma = p_{T\mu}$$

When the invariance group H of $A_{T\mu}$ is nontrivial, the problem of determining the equilibrium states must be supplemented by an analysis of the action of H on \mathcal{M} . Let H_m denote the isotropy group for $m \in \mathcal{M}$, let $0_m = H/H_m$ denote the orbit of m , and let \mathcal{M}_t be the manifold obtained by identifying points of \mathcal{M} belonging to the same orbit. Then,

$$\pi: \mathcal{M} \rightarrow \mathcal{M}_t; m \rightarrow \tilde{m}$$

such that $\pi^{-1}(m) = 0_m$ define a ‘fibration’ of \mathcal{M} over \mathcal{M}_t .⁽¹²⁾ Because $p_{T\mu}$ is invariant under H , it is effectively a function only on \mathcal{M}_t , i.e. there exists a function $\tilde{p}_{T\mu}: \mathcal{M}_t \rightarrow \mathbb{R}$ such that $p_{T\mu} = \tilde{p}_{T\mu} \circ \pi$. The points that minimize $p_{T\mu}$ is expressed by a continuous map

$$\tilde{m}: \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathcal{M}_t; (T, \mu) \mapsto \tilde{m}(T, \mu)$$

The differentiability class of the generating function and thus of the thermostatic statemanifold is determined by the class of the map \tilde{m} . This is easily seen from the definition of the thermostatic pressure

$$p: \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}; (T, \mu) \mapsto p(T, \mu, \tilde{m}(T, \mu))$$

In fact, by successive differentiation of p one sees that p is once more differentiable than \tilde{m} . Moreover, from the definition of \tilde{m} one sees that \tilde{m} is in the worst case piecewise analytic, the analyticity breaking down only along analytic submanifolds, the critical submanifold, that separate the statemanifold in domains, each of which is representing a phase. If the system is undergoing a process described by a curve going from one domain to another, it is said to undergo a phase transition of the second kind.

Phase transitions of the second kind are thus characterized by discontinuities in the thermodynamic quantities obtained by differentiating the generating functions at least twice. However, it might also be associated with other phenomena known as symmetry breaking and topological phase transitions that falls outside the thermostatic description of a system ([9], [10]). To explain these notions, we must consider the subbundle

$$\pi^E: \mathcal{M}^E \rightarrow \mathcal{M}_t^E = \tilde{m}(\mathbb{R}_+ \times \mathbb{R})$$

obtained by restricting the base of $\pi: \mathcal{M} \rightarrow \mathcal{M}_t$ to \mathcal{M}_t^E . \mathcal{M}_t^E is separated into open submanifolds each of which have the same isotropy group. The separating manifold and the boundary contain points with higher dimensional symmetry groups. They are moreover contained in the critical manifold. The thermostatic

⁽¹²⁾ This is a slightly generalized notion of fibration since \mathcal{M}_t might be a manifold with boundary, and the dimension of the fibers might vary.

states can thus be associated with symmetries via the inverse image of m in such a way that all the states of a given phase share the same symmetries described by a subgroup H_p of H . A change of phase might therefore be accompanied by a change of symmetry. If the phase transition reduces the symmetry it is referred to as symmetry breaking.

By the same argument, each phase is associated with an internal statespace isomorphic to H/H_p . The first and second homotopy group of H/H_p gives a classification of the line and point singularities of the states

$$(\eta_\alpha, \phi^\alpha): \mathbb{R}^3 \rightarrow H/H_p$$

by restriction to circles and spheres surrounding the singularities. Since the dynamics is a homotopy, a singularity of a given homotopy class present in the initial condition will be preserved through the evolution if and only if this class is contained in the homotopy group of the internal space of the phase of the final state. A phase transition of the second kind might therefore be accompanied by a change of homotopy groups and thus of the kind of defects that might be present in the equilibrium states. Notice that in the framework of thermostatics that we have exposed, the topological classification of defects has not been used as a characterizing property.

Appendix: Mathematical preliminaries and notation

Let $\mathcal{E} \rightarrow X; (x^i, y^\alpha) \mapsto (x^i)$ denote a fibred manifold with local coordinates $(x^i; y^\alpha)$. We denote by $J_q(\mathcal{E}) \rightarrow X$ its q -jet extension, and by $(x^i; y^\alpha, y_{,i}^\alpha, y_{,i_1 i_2}^\alpha, \dots, y_{,i_1 \dots i_q}^\alpha) = (x^i, y_{\beta_\mu}^\alpha)$ the local coordinates of $J_q(\mathcal{E})$ [2, 4]. Notice that the multi-index $\beta_\mu = (0, i_1, \dots, i_\mu)$ is modulus any permutation of the indices i_1, \dots, i_μ . A q -differentiable section $\gamma: X \rightarrow \mathcal{E}; (x^i) \mapsto (x^i; y^\alpha(x^i))$ can be uniquely prolonged to a section

$$j_q(\gamma): X \rightarrow J_q(\mathcal{E}); (x^i) \mapsto (x^i; y^\alpha(x^i), \partial_{x^i} y^\alpha(x^i), \dots, \partial_{x^{i_1}} \dots \partial_{x^{i_q}} y^\alpha(x^i))$$

Let $f: J_q(\mathcal{E}) \rightarrow \mathbb{R}$ be a differentiable function and γ a $q+1$ -differentiable section $X \rightarrow \mathcal{E}$; the pullback of f by $j_q(\gamma)$ is then a function on X ,

$$f \circ j_q(\gamma): X \rightarrow \mathbb{R}$$

The exterior differential

$$\begin{aligned} d(f \circ j_q(\gamma)) &= \partial_{x^i} f \circ j_q(\gamma) dx^i \\ &= ((\partial_{x^i} + y_{,i}^\alpha \partial_{y^\alpha} + \dots + y_{,i_1 i_2 \dots i_{q+1}}^\alpha \partial_{y_{,i_1 \dots i_q}^\alpha}) f) \circ j_{q+1}(\gamma) dx^i \\ &= (\nabla_i f) \circ j_{q+1}(\gamma) dx^i \end{aligned}$$

The object ∇_i is called the total partial derivative with respect to x^i .

Let $\mathcal{B}(\mathcal{E})$ denote a Banach manifold modelled on \mathcal{E} , i.e. the points of $\mathcal{B}(\mathcal{E})$

can be expressed as section of $\mathcal{E} \rightarrow X$. A function of $f : J_q(\mathcal{E}) \mapsto \mathbb{R}$ by the formula

$$F(\gamma) = \int_{\gamma} f d^n x = \int_X f \circ j_q(\gamma) d^n x$$

iff the integral exists for all $\gamma \in \mathcal{B}(\mathcal{E})$. The exterior differential of a differentiable function $\mathcal{B}(\mathcal{E}) \rightarrow \mathbb{R}$ is a linear form on the vectorfields on $\mathcal{B}(\mathcal{E})$; i.e. $\chi \rightarrow dF(\chi)$ where $dF(\chi)(\gamma)$ is the derivative in the direction χ at γ

$$\begin{aligned} dF(\chi)(\gamma) &= \lim_{t \rightarrow 0} \frac{1}{t} (F(\gamma - t\chi) - F(\gamma)) \\ &= \int_X (\partial_{y_{\beta_\mu}^\alpha} f) \circ j_q(\gamma) \partial_{x^{i_1}} \cdots \partial_{x^{i_\mu}} \chi \circ j_q(\gamma) d^n x \\ &= \int_X (\chi^\alpha \nabla_{y^\alpha} f) \circ j_q(\gamma) d^n x + \text{surface integrals} \end{aligned}$$

where

$$\nabla_{y^\alpha} = (-1)^\mu \nabla_{i_1} \cdots \nabla_{i_\mu} \partial_{y_{\beta_\mu}^\alpha} = \partial_{y^\alpha} - \nabla_i \partial_{y_i^\alpha} + \nabla_i \nabla_j \partial_{y_{ij}^\alpha} - \cdots$$

This indicates that the differential (variational, functional) calculus on $\mathcal{E}(\mathcal{E})$ can be simulated by a differential calculus on $J_q(\mathcal{E})$. We will briefly outline the main aspects of this simulation, and to this end we will give an informal introduction of some objects.

Let $TJ_q(\mathcal{E}) \rightarrow J_q(\mathcal{E})$ denote the tangent bundle of the manifold $J_q(\mathcal{E})$. We denote by $VJ_q(\mathcal{E}) \rightarrow J_q(\mathcal{E})$ and call vertical tangent bundle, the subbundle of $TJ_q(\mathcal{E}) \rightarrow J_q(\mathcal{E})$ defined by the exact sequence

$$0 \rightarrow VJ_q(\mathcal{E}) \rightarrow TJ_q(\mathcal{E}) \rightarrow TX \rightarrow 0$$

The local coordinates of $VJ_q(\mathcal{E})$ are

$$(x^i; y^\alpha, y_{,i}^\alpha, \dots, y_{,i_1 i_2 \dots i_q}^\alpha, v^\alpha, v_{i_1}^\alpha, \dots, v_{i_1 i_2 \dots i_q}^\alpha)$$

Moreover, we will refer to the bundle obtained from the submersion

$$\begin{aligned} VJ_q(\mathcal{E}) &\rightarrow V_r J_q(\mathcal{E}) \\ (x^i; y^\alpha, \dots, v_{i_1 \dots i_q}^\alpha) &\mapsto (x^i; y^\alpha, \dots, y_{,i_1 \dots i_q}^\alpha, v^\alpha) \end{aligned}$$

as the reduced vertical tangent bundle. The symbol χ of a vectorfield of $\mathcal{B}(\mathcal{E})$ can be represented as a section

$$J_q(\mathcal{E}) \rightarrow V_r J_q(\mathcal{E}); (x^i; y_{\beta_\mu}^\alpha) \mapsto (x^i; y_{\beta_\mu}^\alpha, \chi^\alpha(x^i; y_{\beta_\mu}^\alpha))$$

We denote by $V^* J_q(\mathcal{E})$ the dual bundle of $VJ_q(\mathcal{E})$. It is the vertical cotangent bundle. A section a of $V^* J_q(\mathcal{E})$ is a vertical 1-form on $J_q(\mathcal{E})$

$$a = a_\alpha dy^\alpha + a_{i_1}^\alpha dy_{i_1}^\alpha + \cdots + a_{i_1 \dots i_q}^{\beta_q} dy_{i_1 \dots i_q}^{\beta_q}$$

We can define an action of a on the sections of $V_r J_q(\mathcal{E}) \rightarrow J_q(\mathcal{E})$ by the formula

$$a(\rho_q(\chi)) = a_\alpha \chi^\alpha + a^i \nabla_i \chi^\alpha + \cdots + \alpha^{\beta_q} \nabla_{i_1} \cdots \nabla_{i_q} \chi^\alpha$$

when $\rho_q(\chi)$ denotes the q -prolongation of χ ,

$$\rho_q(\chi) = (\chi^\alpha, \nabla_i \chi^\alpha, \dots, \nabla_{i_1} \cdots \nabla_{i_q} \chi^\alpha)$$

Considered as an integrand, $a(\rho_q(\chi))$ is equivalent to

$$(a_\alpha - \nabla_i a_\alpha^i + \nabla_i \nabla_j a_\alpha^{ij} + \cdots + (-1)^q \nabla_{i_1} \cdots \nabla_{i_q} a_\alpha^{\beta_q}) \chi^\alpha = \bar{a}_\alpha \chi^\alpha$$

via a number of partial integrations, assuming χ^α to have been given boundary conditions such that the surface integrals vanishes. This shows that a 1-form on $\mathcal{B}(\mathcal{E})$ can be represented by either of the symbols $a_\alpha^{\beta_\mu} dy_{\beta_\mu}^\alpha$ or $\bar{a}_\alpha dy^\alpha$. We notice that when the coefficients $a_\alpha^{\beta_\mu}$ are functions on $J_q(\mathcal{E})$, the coefficients a_α are functions on $J_{2q}(\mathcal{E})$, having a particular polynomial dependence on the variables $y_{,i_{q+1}}^\alpha, \dots, y_{,i_{2q}}^\alpha$. We will call reduced vertical cotangent bundle and denote by $V_r^* J_{2q}(\mathcal{E}) \rightarrow J_{2q}(\mathcal{E})$ the bundle in which $\bar{a}_\alpha dy^\alpha$ is naturally represented as a section. Its canonical coordinates will be denoted $(x^i; y^\alpha, \dots, y_{,i_1 \dots i_{2q}}^\alpha, z_\alpha)$. There exists a canonical 1-form $\theta = z_\alpha dy^\alpha$ on $V_r^* J_{2q}$ which is 'equivalent' to the canonical 1-form $\Theta = u_\alpha dy^\alpha + \cdots + u_\alpha^{i_1 \dots i_q} dy_{,i_1 \dots i_q}^\alpha$ on $V^* J_q(\mathcal{E})$. Since each fiber of $V^* J_q(\mathcal{E}) \rightarrow X$ possesses a symplectic structure $d\Theta$ called a vertical symplectic structure of $V^* J_q(\mathcal{E}) \rightarrow X$, we can introduce the notion of a vertical Lagrangian submanifold of $V^* J_q(\mathcal{E})$.

Definition. Let M be a manifold of dimension half the dimension of the fibers of $V^* J_q(\mathcal{E}) \rightarrow X$, and let $\phi_x, x \in X$ be a family of embeddings

$$\phi_x : M \rightarrow V^* J_{qx}(\mathcal{E})$$

then $L = \phi_x(M) \subset V^* J_q(\mathcal{E})$ is called a vertical Lagrangian submanifold if

$$d(\theta | L) = 0$$

Thus, the graph of a closed 1-form is an example of a vertical Lagrangian submanifold in this setting, the generatization being merely that we do not assume that the projection of L on $J_q(\mathcal{E})$ is non-singular. As for the 1-form 'L' can be equivalently represented by a submanifold l of $V_r^* J_{2q}(\mathcal{E})$. In this case the Lagrangian condition is expressed by $d(\theta | l) = 0$, because the 'vertical' exterior derivative commutes with the partial integration procedure which permits us to go from one representation to the other.

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