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On the equations of motion of an N-component charged fluid

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Abstract. We construct equations of motion for a fluid consisting of N charged chemical components. The basic assumption is that the dynamical vectorfield is the sum of two terms: a 'conservative' term, being a Hamiltonian vectorfield associated with the energy function of the system; and a 'dissipative' term, being a gradient vectorfield associated with a family of functions. The resulting equations conforms to the standard expressions for the equations of motion for such systems.

1. Introduction

According to the laws of thermodynamics, a thermodynamic system is defined by giving one of the thermodynamic potentials referred to as the energy $\hat{u}$, the free energy $\hat{f}$ or the entropy $\hat{s}$. The theory contains the prescription for the construction of any of the other two potentials once one of them is known. These laws tell us moreover, that the entropy of an isolated system is monotonically increasing during the evolution. Isolated means here that the system is thermally and mechanically isolated and that there are no external fields. The total energy, total momentum etc. are thus constants of motion. Clearly, the information about the nature of the dynamics contained in the laws of thermodynamics is rather limited. It tells essentially only that it is not a Hamilton dynamics; the dynamical vectorfield χ could however, be a gradient field.

A study of books and papers on thermodynamics [1, 2, 3], reveals that χ is always taken to be the sum of two terms: A Hamiltonian vectorfield χ^H defined by the energy function and leaving the entropy invariant, and a vectorfield χ^G describing the directed transformation of mechanical and other forms of energy into heat. Much less is 'known' about the structure of χ^G than of χ^H. One assumes only that some of its components must have a certain form. In this paper we will show that these conditions are compatible with the assumption that χ^G is a gradient vectorfield constructed from a family of functions $\tilde{r}$, the dissipation function.

The information that goes into the dissipation function is assumed to be

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contained, partly in a map ψ and partly in a function r. ψ which is assumed to be a submersion describes the dissipation mechanisms that are generally valid physical laws while r contains the information about the dissipation coefficients of the particular system under consideration. The dissipation function is then given as $r = r \circ \psi$.

The complete information about the dynamics of a thermodynamic system could thus be contained in two functions u and r and a map ψ, where moreover, ψ is the same for a whole class of systems. It is clear that if this is true, then the task of determining workable models by successive trial and error, guesses and experiments, is much simplified. In particular, models simulating the behaviour of systems close to critical points are more easily obtained due to the results of singularity theory and catastrophe theory which limits the number of possible models. From a more theoretical point of view, the additional structure imposed on thermodynamics by our assumptions and constructions, might become a study of its own. In fact, one can probably make statements about the dynamics that are valid for general u and r or classes of u and r. As concerns ψ, it should be the object of a study of its own. It may be related to invariance properties under group actions, and its study may thus a priori be completely dissociated from dynamical considerations.

Our main motivation for this study has however, been the construction of a dynamics for multi component systems. Not only does the combinatorial possibilities introduce complications when one tries to establish the equations of motion for such systems 'by hand' (establish the equations of motion for the 3-body celestial mechanics problem using Newton's laws and the law of attraction and compare with the derivation using the methods of hamiltonian or lagrangian mechanics), but we do not even have any clear idea of what would be the analog to Newton's laws when we have mutual interactions between fluid components. The methods employed in this paper presents a possible solution to these problems. Due to the different nature of the variables of different classes of thermodynamic systems, it is not very convenient to give the general theory. We have thus chosen to consider the class of N-component charged fluids. The theory is general enough to admit systems described by energy density functions that depend, not only on the extensive variables, but except for the entropy density, also on their derivatives to the order q.

The state space of a thermodynamic system is a Banach manifold $\mathcal{B}(\mathscr{E})$, being represented as a function space over space $X = \mathbb{R}^3$. The states thus are sections $\gamma: X \to \mathscr{E}$ of a fibred manifold $\pi: \mathscr{E} \to X$. Moreover, the extensive observables of the system being functions $F: \mathcal{B}(\mathscr{E}) \to \mathbb{R}$, are represented as integrals $\gamma \to F(\gamma) = \int_\gamma f\, d^3x$, where $f: J_q(\mathscr{E}) \to \mathbb{R}$ is a function on the q-jet extension $\mathscr{J}_q(\mathscr{E})$ of $\mathscr{E}$, i.e. of γ and its derivatives up to order q. Now, given $\mathscr{E}$, $\mathscr{J}_q(\mathscr{E})$ is canonically given; moreover, $\mathscr{J}_q$ is a functor, thus morphisms of $\mathscr{E}$ are lifted by $\mathscr{J}_q$ to morphisms of $\mathscr{J}_q(\mathscr{E})$ [4]. There also exist functors $\mathcal{B}$ between the category of fibred manifolds and the category of Banach manifolds [5]. However, presently one does not know which one to choose, i.e. which topology to choose on $\mathcal{B}(\mathscr{E})$ in thermodynamics. Whatever this might be a main part of thermodynamics can be formulated and a number of formal properties can be studied using the standard methods of differential calculus on $\mathscr{E}$ and $\mathscr{J}_q(\mathscr{E})$. This is what we will do in the following. A brief exposition of these methods, and the notation we will use is found in an appendix to this paper.

To give a detailed account of the content of this paper, we will briefly describe the construction of χ^H and χ^G for a one component system associated with an energy density function u that does not depend on the derivatives of the extensive density variables, i.e.

$$u: \mathscr{E} \rightarrow \mathbb{R}; \qquad (x^i, s, \pi_i, \rho, B^i, D^i) \mapsto u(x^i, s, \pi_i, \rho, B^i D^i)$$

The assumption is that 'all' information contained in χ^H is already contained in u. It is well known that the hamiltonian vectorfield constructed for the conjungate variables (w, ρ), (Φ, s), (D^i, A_i) and related to the extensive variables by

$$\pi_i = \rho \nabla_i w + s \nabla_i \Phi - \lambda \rho A_i$$
$$B^i = \varepsilon^{ijk} \nabla_j A_k$$

satisfy the conditions that one puts on χ^H a priori. In fact, it leaves invariant the energy, momentum and mass, and moreover, conserves the constraints $\nabla_i D^i - \lambda\rho = 0$ and $\nabla_i B^i = 0$. Computing χ^H one finds

$$\begin{aligned}
\chi^H(\rho) &= \nabla_w u(x^i, s, \rho\nabla_i w + s\nabla_i\Phi - \lambda\rho A_i, \rho, D^i, \varepsilon^{ijk}\nabla_j A_k) \\
&= -\nabla_j(\rho v^i(\,.\,.)) \\
\chi^H(w) &= -\nabla_\rho u(\,.\,.) = -v^i(\,.\,.)\nabla_i w - \mu(\,.\,.) + \lambda A_i v^i \\
\chi^H(s) &= \nabla_\Phi u(\,.\,.) = -\nabla_i(s v^i(\,.\,.)) \\
\chi^H(\Phi) &= -\nabla_s u(\,.\,.) = -v^i(\,.\,.)\nabla_i \Phi - T(\,.\,.) \\
\chi^H(D^i) &= \nabla_{A_i} u(\,.\,.) = \varepsilon^{ijk}\nabla_j H_k(\,.\,.) - \lambda\rho v^i(\,.\,.) \\
\chi^H(A_i) &= -\nabla_{D^i} u(\,.\,.) = -E^i(\,.\,.)
\end{aligned}$$

where $\nabla_w = \partial_w - \nabla_i\, \partial_{\nabla_i w}$ etc. denotes the 'functional derivative', $v^i(\,.\,.) = \partial_{\pi_i} u(\,.\,.)$, $\mu(\,.\,.) = \partial_\rho u(\,.\,.)$, $H_i(\,.\,.) = \partial_{B^i} u(\,.\,.)$ and $E^i(\,.\,.) = \partial_{D^i} u(\,.\,.)$. Thus, for example, $\chi^H(\pi_i)$ is obtained from

$$\begin{aligned}
\chi^H(\rho\nabla_i w + s\nabla_i\Phi - \lambda\rho A_i) &= \chi^H(\rho)\nabla_i w + \chi^H(\nabla_i w)\rho \\
&+ \chi^H(s)\nabla_i\Phi + \chi^H(\nabla_i\Phi)s - \lambda\chi^H(\rho)A_i - \lambda\chi^H(A_i)\rho
\end{aligned}$$

Computing this expression and changing variables one obtains

$$\begin{aligned}
\chi^H(\pi_i + \varepsilon_{ijk}B^j D^k) &= -\nabla_j t_i^j \\
&= -\nabla_j\{\pi_i v^j - E_i D^j - H_i B^j + \delta_i^j(-u + \pi_k v^k + \mu\rho + E_k D^k + H_k B^k)\}
\end{aligned}$$

The computation of the stress tensor t_i^j depends on the assumption that u does not depend on x^i explicitly. This assumption and the assumption that u is invariant under rotations are naturally imposed on energy function densities describing isolated systems. The invariance condition implies that $\delta^{ik}t^j_k$ is symmetric in the indices ij, and thus that the angular momentum is conserved. Notice that the linear dependence of π_i on A_i in the dynamical variables is necessary in order to conserve the constraint $\nabla_i D^i - \lambda\rho = 0$.

The vectorfield χ^H leaves invariant the entropy and does thus not satisfy the Second Law. In fact, no hamiltonian vectorfield could, since hamiltonian vectorfields do not possess attractors. We must therefore add to χ^H a vectorfield χ^G that is transverse to the equi-entropy submanifolds and tangent to the equi-energy, equi-charge, equi-momentum, equi-mass and equi-angular momentum submanifolds. This is not enough however. It can be shown that χ^H constructed above is zero on the extrema of the entropy in the constant charge, energy, momentum and mass submanifolds and thus also on its maxima. χ^G must have these maxima as attractors.

To construct χ^G we will first consider the conditions determining the extrema of the entropy in the submanifolds of given energy, momentum and mass.[2]) These are partly determined by the zeroes of the first derivatives (variations) of the entropy with respect to vectorfields tangent to the above mentioned submanifolds. The result is

$$\nabla_i\, \partial_u s(x^i, u, \pi_i, \rho) = 0$$
$$\nabla_i\, \partial_{i\pi_k} s(\ldots) + \zeta_{ij}\zeta^{kl}\nabla_l\, \partial_{\pi j} s(\ldots) = 0$$
$$\nabla_i\, \partial_{i\rho} s(\ldots) = 0$$

Together with a further extremal condition obtained by variation with local deformations, we possess a complete set of extremal conditions for the entropy and are able to show that the extrema of the entropy are equilibrium points for χ^H. Returning to our immediate problem, we see that if we let $\tilde{r}$ be a family of functions parametrised by the intensive variables, of the extremal conditions given above,

$$\tilde{r}(\,.\,.\,)(\nabla_i\beta,\ \nabla_i\Omega^j,\ \nabla_i\nu)$$

where $\beta = \partial_u s(\,.\,.\,)$ etc., then, automatically χ^G defined by

$$\chi^G(u) = \nabla_\beta \tilde{r} = -\nabla_i\, \partial_{\nabla_i\beta}\tilde{r}$$
$$\chi^G(\pi_i) = \nabla\pi_i \tilde{r} = -\nabla_i\, \partial_{\nabla_j\Omega^i}\tilde{r}$$
$$\chi^G(\rho) = \nabla_\rho \tilde{r} = -\nabla_i\, \partial_{\nabla_i\nu}\tilde{r}$$

are tangent to the equi-energy, equi-momentum and equi-mass submanifolds. Moreover if we assume that $\tilde{r}_{(\,.\,.\,)}$ depends on the "squares" of the extremal conditions, χ^G is zero on the extremal states of the entropy. The direction of the evolution is expressed by a condition on r. It turns out however, that in order to have a vectorfield χ^G that leaves invariant the angular momentum also, we must

[2]) We assume for simplicity that we have no charge and no fields.

put further conditions on $\tilde{r}_{(..)}$. In fact, $\tilde{r}_{(..)}$ can depend only on certain combinations of the extremal conditions. In other words,

$$\tilde{r}_{(..)} = r_{(..)} \circ \psi$$

where ψ express the map defining these combinations. References to the literature on the subject can be found in [6].

2. Definition of the system

The local observables of an N-component charged fluid are functions on the q-jet extension $\mathscr{J}_q(\mathscr{E})$ of the fibred manifold

$$\mathscr{E}_u = \{(x^i, s_n, \pi_{ni}, \rho_n, D^i, B^i) \in \mathbb{R}^3 \times \mathbb{R}_+^N \times \mathbb{R}^{3N} \times R_+^N \times \mathbb{R}^3 \times \mathbb{R}^3\}$$

where the fibration is defined by

$$\mathscr{E}_u \to X; \qquad (x^i, s_n, \pi_{ni}, \rho_n, D^i, B^i) \mapsto (x^i)$$

i.e.

$$\mathscr{J}_q(\mathscr{E}_u) \to \{(x^i, s_n, \ldots, B^i, s_{n,i}, \ldots, B^i_{,i}, \ldots, s_{n,i_1 \cdots i_q}, \ldots, B^i_{,i_1 \cdots i_q})\}$$

Thus, the extensive local observables of entropy-density s_n, momentum-density π_{n_i} and mass density ρ_n of the nth component, electric displacement D^i and magnetic polarization B^i are represented by the functions $\mathscr{J}_q(\mathscr{E}_u) \to \mathbb{R}$

$$\hat{s}_n(x^i, s_n, \ldots) = s_n$$
$$\hat{\pi}_{ni}(\ldots) = \pi_{ni}$$
$$\hat{\rho}_n(\ldots) = \rho_n$$
$$\hat{D}^i(\ldots) = D^i$$
$$\hat{B}^i(\ldots) = B^i$$

By construction, these function constitutes a set of coordinate functions for the fibers of $\mathscr{E}_u$. We will however, also need to consider the local extensive observables of total entropy density, total momentum density j_i, total mass density ρ, total angular momentum density l_i and total charge density q which are given by the functions

$$\hat{s}(\ldots) = \sum_{n=1}^{N} s_n$$

$$\hat{j}_i(\ldots) = \sum_{n=1}^{N} \pi_{ni} + \varepsilon_{ijk} D^j B^k$$

$$\hat{\rho}(\ldots) = \sum_{n=1}^{N} \rho_n$$

$$\hat{l}_i(\ldots) = \varepsilon_{ijk}\delta^{kl}x^j\hat{j}_l(\ldots)$$

$$\hat{q}(\ldots) = \sum_{n=1}^{N} \lambda_n \rho_n$$

where ε and δ are the usual summation symbols and λ_n is the unity of charge on unity of mass of the nth component.

It is assumed that the constraints

$$\hat{\alpha} = 0 \quad \text{and} \quad \hat{a} = 0$$

are satisfied for

$$\hat{\alpha} : \mathscr{J}_1(\mathscr{E}_u) \to \mathbb{R},\ (.) \mapsto D^i_{,i} - \sum_{n=1}^{N} \lambda_n \rho_n$$

$$\hat{a} : \mathscr{J}_1(\mathscr{E}_u) \to \mathbb{R},\ (.) \mapsto B^i_{,i}$$

The constraints express two of Maxwell's equations.

According to the laws of thermodynamics, a thermodynamic system is uniquely defined by its energy function, i.e. in this setting by the energy-density $\hat{u}$

$$\hat{u} : \mathscr{J}_q(\mathscr{E}_u) \to \mathbb{R}$$

If the system is *isolated,* then $\hat{u}$ is homogeneous i.e. $\partial_{x^i}\hat{u} = 0$, and invariant under rotations. In any case, we assume that $\hat{u}$ does not depend on the derivatives of s_n, $\nabla s_n \hat{u} = \partial s_n \hat{u}$.[3])

To a given set of extensive observables we have a corresponding set of intensive local observables. In the given representation these are the temperature T_n, the velocity v^i_n and chemical potential μ_n of the nth component, the electric field strength E_i and the magnetic field strength H_i. They are represented by the functions $\mathscr{J}_q(\mathscr{E}_n) \to \mathbb{R}$

$$\hat{T}_n(.) = \partial_{s_n}\hat{u}(.)$$

$$\hat{v}^i(.) = \nabla_{\pi_{ni}}\hat{u}(.)$$

$$\hat{\mu}_n(.) = \nabla_{\rho_n}\hat{u}(.)$$

$$\hat{E}_i(.) = \nabla_{D^i}\hat{u}(.)$$

$$\hat{H}_i(.) = \nabla_{B^i}\hat{u}(.)$$

for a system described by the energy density function $\hat{u}$. $\hat{u}$ is said to be the potential function in this representation called the energy representation.

Since $\hat{T}_n = \partial_{s_n}\hat{u} > 0$, the map

$$\varphi_{us} : \mathscr{J}_q(\mathscr{E}_u) \to \mathscr{J}_q(\mathscr{E}_s)$$

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[3]) $\nabla_s = \partial_s - \nabla_i \partial_{s_{,i}} + \nabla_i \nabla_j \partial_{s_{,ij}} \cdots$

where

$$\mathscr{E}_s = \{(x^i, u, \sigma_m, \pi_{ni}, \rho_n, D^i, B^i) \in \mathbb{R}^3 \times \mathbb{R} \times \mathbb{R}^{N-1} \times \cdots \times \mathbb{R}^3\}$$

$$\sigma_m = \sum_{n=1}^{m} s_n \qquad m = 1, \ldots, N-1$$

is a diffeomorphism. On $\mathscr{E}_s$, u appears as a coordinate function and s as a potential function.

3. The dynamics

The evolution of a thermodynamic system during a time interval $[t_0, t_1]$ is described by a curve c on the state-space $\mathscr{B}(\mathscr{E})$. c is a generalized solution of an ordinary differential equation on $\mathscr{B}(\mathscr{E}_u)$, the equation of motion

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

where χ denote the symbol for the dynamical vectorfield on $\mathscr{B}(\mathscr{E})$. $\chi = \chi^\alpha \nabla_{y\alpha}$ is represented as a differential operator on $\mathscr{J}_q(\mathscr{E})$, its coefficients χ^α are functions on $\mathscr{J}_q(\mathscr{E})$.

The only explicit assumption on the dynamics usually given is the following version of the Second Law of Thermodynamics:

$$\int_{c(t_2)} \tilde{s} \geqslant \int_{c(t_1)} \tilde{s}, \qquad \forall t_2 > t_1$$

i.e., the entropy is a Lyapounov function for the evolution c of an isolated system. However, if one looks at standard formulations of thermodynamics, one finds that these satisfiy stronger requirements. For example:

The Dynamical Postulate. The dynamics of an isolated system is supposed to be described by a vectorfield χ such that

(a) $\chi = \chi^H + \chi^G$ with

$$\chi^H(\hat{s}) = \nabla_i \zeta_s^{Hi} \quad \text{and} \quad \int_\gamma \chi^G(s) \geqslant 0$$

(b) (1) $\chi^H(\hat{u}) = \nabla_i \zeta_u^{Hi}$ and $\chi^G(\hat{u}) = \nabla_i \zeta_u^{Gi}$
(2) $\chi^H(\hat{j}_i) = \nabla_k \zeta_{ji}^{Hk}$ and $\chi^G(\hat{j}_i) = \nabla_k \zeta_{ji}^{Gk}$
(3) $\chi^H(\hat{\rho}) = \nabla_i \zeta_\rho^{Hi}$ and $\chi^G(\hat{\rho}) = \nabla_i \zeta_\rho^{Gi}$
(4) $\chi^H(\hat{B}^i) = \varepsilon^{ijk} \nabla_j \zeta_{Bk}^H$ and $\chi^G(\hat{B}^i) = \varepsilon^{ijk} \nabla_j \zeta_{Bk}^G$
(5) $\chi^H(\hat{q}) = \nabla_i \zeta_q^{Hi}$ and $\chi^G(\hat{q}) = \nabla_i \zeta_q^{Gi}$
(6) $\delta^{il} \zeta_{jl}^{Hk} = \delta^{kl} \zeta_{jl}^{Hi}$ and $\delta^{il} \zeta_{jl}^{Gk} = \delta^{kl} \zeta_{jl}^{Gi}$
(7) $\chi^H(\hat{q}) = \nabla_i \chi^H(\hat{D}^i)$ and $\chi^G(\hat{q}) = \nabla_i \chi^G(\hat{D}^i)$

The conditions under (a) express that the dynamical vectorfield can be written 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 terms are vectorfields for which the energy (1), the total momentum (2), the total mass (3), the magnetic flux through any closed surface (4), the total charge (5), the total angular momentum and the constraint function $\hat{\alpha}$ (7) are conserved. Clearly, given a priori a dynamical vectorfield χ these conditions may not determine a unique separation of χ into two terms satisfying the conditions under a) and b). In the following we will however, "construct" a dynamical vectorfield χ that satisfies these conditions, by constructing χ^H and χ^G separately.

4. The Hamiltonian term χ^H

Let $\tilde{\mathscr{E}}$ be the fibred manifold

$$\tilde{\mathscr{E}} = \{(x^i, w_n, \rho_n, \phi_n, s_n, D_i, A_i)\varepsilon \cdots\} \to X = \{(x^i) \in \mathbb{R}^3\}$$

and let ω be the symplectic form on the fibres

$$\omega = \sum_{n=1}^{N} (dw_n \wedge d\rho_n + d\phi_n \wedge ds_n) + dD^i \wedge dA_i$$

Moreover, denote by Φ the submersion

$$\mathscr{J}_1(\tilde{\mathscr{E}}) \to \mathscr{E}_u$$

$$(x^i, w_n, \rho_n, \phi_n, s_n, D^i, A_i, w_{n,i}, \rho_{n,i}, \phi_{n,i}, \ldots, A_{i,j})$$
$$\mapsto (x^i, s_n, \rho_n w_{n,i} + s_n \phi_{n,i} - \lambda_n \rho_n A_i, \rho_n, D^i, \varepsilon^{ijk} A_{j,k})$$

The Hamiltonian of a system is by assumption the density

$$\hat{h} = \hat{u} \circ \mathscr{J}_q(\Phi) : \mathscr{J}_{q+1}(\tilde{\mathscr{E}}) \to \mathbb{R}$$

obtained by taking the pullback of its energy-density

$$\hat{u} : \mathscr{J}_q(\mathscr{E}_u) \to \mathbb{R}$$

Proposition. *The pushforward under Φ of the Hamiltonian vectorfield $(-\nabla_{\rho_n}\hat{h}, \nabla_{w_n}\hat{h}, -\nabla_{s_n}\hat{h}, \nabla_{\phi_n}h, \nabla_{A_i}\hat{h}, -\nabla_{D_i}\hat{h})$ is the vectorfield χ^H whose components are*

$$\chi^H(\hat{s}_n) = -\nabla_i(s_n \nabla_{\pi_{ni}} \hat{u})$$

$$\chi^H(\hat{\pi}_{ni}) = -\nabla_j(\pi_{ni} \nabla_{\pi_{ni}} \hat{u}) - \rho_n \nabla_i \nabla_{\rho_n} \hat{u} - \pi_{nj} \nabla_i \nabla_{\pi_{nj}} \hat{u}$$
$$- s_n \nabla_i \nabla_{s_n} \hat{u} + \lambda_n \rho_n \nabla_{D^i} \hat{u} + \varepsilon_{ijk} \lambda_n \rho_n \nabla_{\pi_{nj}} \hat{u} B^k$$

$$\chi^H(\hat{\rho}_n) = -\nabla_i(\rho_n \nabla_{\pi_{ni}} \hat{u})$$

$$\chi^H(\hat{D}^i) = \varepsilon^{ijk} \nabla_j \nabla_{B^k} \hat{u} - \sum_{n=1}^{N} \lambda_n \rho_n \nabla_{\pi_{ni}} \hat{u}$$

$$\chi^H(\hat{B}^i) = -\varepsilon^{ijk} \nabla_j \nabla_{D^k} \hat{u}$$

Proof. The proposition is proved by direct computation using the formulae of Paragraph 8. ■

Theorem. *The vectorfield χ^H computed above satisfies the conditions of the dynamical postulate.*

Proof. (a) is automatically satisfied since s is a constant of motion for χ^H. (b) is proved by computation and inspection, thus

$$(1)\ \chi^H(\hat{u}) = -\nabla_i\left\{\sum_{n=1}^{N}(s_n\nabla_{s_n}\hat{u} + \pi_{nj}\nabla_{\pi_{nj}}\hat{u} + \rho_n\nabla_{\rho_n}\hat{u})\nabla_{\pi_{ni}}\hat{u} + \varepsilon^{ijk}\nabla_{D^j}\hat{u}\nabla_{B^k}\hat{u}\right\} = \nabla_i\zeta_u^{Hi}$$

$$(2)\ \chi^H(\hat{j}_i) = -\nabla_i\left\{\sum_{n=1}^{N}(\pi_{ni}\nabla_{\pi_{nj}}\hat{u}) + P_i^j - D^j\nabla_{D^i}\hat{u} - B^j\nabla_{B^i}\hat{u} + \delta_i^j\left(-\hat{u} + \sum_{n=1}^{N}(\pi_{nk}\nabla_{\pi_{nk}}\hat{u} + \rho_n\nabla_{\rho_n}\hat{u} + s_n\nabla_{s_n}\hat{u}) + D^k\nabla_{D^k}\hat{u} + B^k\nabla_{B^k}\hat{u}\right)\right\} = \nabla_k\zeta_{ji}^{Hk}$$

where P_i^j is a solution of the equation

$$\nabla_j P_i^j = \sum_{n=1}^{N}(s_n\nabla_i\,\partial_{s_n}\hat{u} + \pi_{nk}\nabla_i\nabla_{\pi_{nk}}\hat{u} + \rho_n\nabla_i\nabla_{\rho_n}\hat{u}) + D^k\nabla_i\nabla_{D^k}\hat{u} + B^k\nabla_i\nabla_{B^k}\hat{u} - \nabla_i\Big(-\hat{u} + \sum_{n=1}^{N}(s_n\,\partial_{s_n}\hat{u} + \pi_{nk}\nabla_{\pi_{nk}}\hat{u} + \rho_n\nabla_{\rho_n}\hat{u}) + D^k\nabla_{D^k}\hat{u} + B^k\nabla_{B^k}\hat{u}\Big)$$

i.e. $P = P_\pi + P_\rho + P_D + P_B$ where each term looks like

$$\begin{aligned} &p_i\,\partial_{p_j}\hat{u} \\ &+ p_{ii_1}\,\partial_{p_{i_1}}\hat{u} - p_i\nabla_{i_1}\,\partial_{p_{i_1j}}\hat{u} \\ &+ p_{ii_1i_2}\,\partial_{p_{i_1i_2j}}\hat{u} - p_{ii_1}\nabla_{i_2}\,\partial_{p_{i_1i_2j}}\hat{u} + p_i\nabla_{i_1}\nabla_{i_2}\,\partial_{p_{i_1i_2j}}\hat{u} \\ &\quad\cdot \\ &\quad\cdot \\ &\quad\cdot \\ &+ p_{ii_i\cdots i_{q-1}}\,\partial_{p_{ii_1\cdots i_{q-1}}}\hat{u} - \cdots (-1)^{q-1}p_i\nabla_{i_1}\cdots\nabla_{i_{q-1}}\,\partial_{p_{i_1\cdots i_{q-1}j}}\hat{u} \end{aligned}$$

$$(3)\ \chi^H(\hat{\rho}) = -\nabla_i\sum_{n=1}^{N}\rho_n\nabla_{\pi_{ni}}\hat{u} = \nabla_i\zeta_\rho^{Hi}$$

$$(4)\ \chi^H(\hat{B}^i) = -\varepsilon^{ijk}\nabla_j\nabla_{D^k}\hat{u} = \varepsilon^{ijk}\nabla_j\zeta_{Bk}^H$$

$$(5)\ \chi^H(\hat{q}) = -\nabla_i\sum_{n=1}^{N}\lambda_n\rho_n\nabla_{\pi_{ni}}\hat{u} = \nabla_i\zeta_q^{Hi}$$

(6) holds because $\hat{u}$ is invariant under rotations and thus a function of elementary invariants only.
(7) holds. ■

The vectorfield χ^H is a generalization of the Euler–Maxwell vectorfield for a one-component charged fluid [2]. In fact, if $n = 1$ and $\hat{u} : \mathscr{E}_u \to \mathbb{R}$ is of the form

$$\hat{u}(s, \pi_i, \rho, D^i, B^i) = \frac{\delta^{ij}\pi_i\pi_j}{2\rho} + \hat{u}_0(s, \rho, D^i, B^i)$$

then the velocity $v^i = \delta^{ij}\pi_j/\rho$, and

$$\chi^H(v^i) = -v^j\nabla_j v^i + \delta^{ij}(E_j + \varepsilon_{jk1}v^k B^1) - \frac{1}{\rho}\nabla_j\hat{p}$$

where $E_i = \partial_{D^i}\hat{u}_0$ and $\hat{p} = -\hat{u}_0 + s\,\partial_s\hat{u}_0 + \rho\,\partial_\rho\hat{u}_0$.

As another piece of justification of χ^H we will show that the momentum-flux-density tensor is the *stress tensor,* i.e. the 'intensive variable' for the deformation tensor. Thus, let φ_t, $\tau \in (-\varepsilon, \varepsilon)$ be a flow on $\mathbb{R}^3$. It is said to define a deformation by the map

$$\phi_\tau : \mathscr{E}_u \to \mathscr{E}_u, (s_n, \pi_{ni}, \rho_n, D^i, B^i) \mapsto (j(\varphi_\tau)s_n \circ \varphi_\tau, j(\varphi_\tau)\,\partial_x i\varphi^j_\tau\pi_{nj} \circ \varphi_\tau$$
$$j(\varphi_\tau)\rho_n \circ \varphi_\tau, j(\varphi_\tau)(\partial_{x^j}\varphi^i_\tau)^{-1}D^j \circ \varphi_\tau, j(\varphi_\tau)(\partial_{x^j}\varphi^i_\tau)^{-1}B^j \circ \varphi_\tau)$$

where $j(\varphi_\tau)$ denotes the jacobian determinant of φ_τ. The generator of ϕ_τ is easily determined, it is given by the vectorfield

$$(\nabla_i(s_n\xi^i), \pi_{nj}\nabla_i\xi^j + \nabla_i(\pi_{nj}\xi^i), \nabla_i(\rho_n\xi^i), -D^j\nabla_j\xi^i + \nabla_j(D^i\xi^j),$$
$$-B^j\nabla_j\xi^i + \nabla_j(B^i\xi^j)$$

where ξ is the generator of φ_τ. A deformation of $\hat{u}$ is a derivation in the direction of the above vectorfield. A computation shows that it is given by

$$-\xi^i\nabla_k\zeta^{Hk}_{ji}$$

Notice that we have assumed that ξ^i is tangent to the boundary of $\mathscr{D}$ i.e. $\varphi_\tau(\partial\mathscr{D}) = \partial\mathscr{D}\ \forall\tau \in [-\varepsilon, \varepsilon]$.

5. The equilibrium conditions

The equilibrium conditions for a given system are the conditions determining the maxima of its entropy with respect to a certain class of variations τ. The conditions fall into two classes, the extremum conditions and the maximum or stability conditions, which will not be discussed here. The extremum conditions express that the entropy is extremal with respect to the variations by local deformations, and with respect to the variations, that leave invariant the total energy, the total momentum, the total mass, the total angular momentum, the total charge, the total magnetic flux through any closed surface, and the constraint function α.

The local deformations are generated by vectorfields of the form

$$(\nabla_i(u\xi^i),\ \pi_{nj}\nabla_i\xi^j + \nabla_i(\pi_{nj}\xi^i),\ \nabla_i(\sigma_n\xi^i),\ \nabla_i(\rho_n\xi^i),\ -D^i\nabla_i\xi^j + \nabla_i(D^j\xi^i),$$
$$-B^i\nabla_i\xi^j + \nabla_i(B^j\xi^i))$$

where ξ^i is a vectorfield on $X = \mathbb{R}^3$ tangent to $\partial\mathcal{D}$, the boundary of $\mathcal{D}$. To specify the other vector fields belonging to the class τ, it is convenient to introduce coordinates corresponding to the conserved quantities. This is accomplished by the following diffeomorphism

$$\mathscr{E}_s \to \mathscr{E}_s$$
$$(u, \pi_{ni}, \sigma_n, \rho_n, D^i, B^i) \to (u, j_i, p_{mi}, q, \rho, \sigma_n, \eta_n, D^i, B^i)$$

where j_i, q and ρ has been defined already and

$$p_{mi} = \frac{\sum_{\alpha=1}^{m} \rho_\alpha \pi_{m+1} - \rho_{m+1} \sum_{\alpha=1}^{m} \pi_\alpha}{\sum_{\alpha=1}^{m} \rho_\alpha}$$

$$\eta_n = \sum_{m=1}^{n} \rho_{m+1}$$

One then verifies easily that the vectorfields χ with components of the form

$$\chi(\hat{u}) = \nabla_i \zeta_u^i$$
$$\chi(\hat{j}_i) = \nabla_k \zeta_{ji}^k + \zeta_{ki}\zeta^{ml}\,\nabla_m \zeta_{jl}^k$$
$$\chi(\hat{p}_{mi}) = \chi_{p_{mi}}$$
$$\chi(\hat{q}) = \nabla_i \zeta_q^i$$
$$\chi(\hat{\rho}) = \nabla_i \zeta_\rho^i$$
$$\chi(\hat{\eta}_n) = \chi_{\eta_n}$$
$$\chi(\hat{D}^i) = \zeta_q^i + \varepsilon^{ijk}\nabla_j \psi_k$$
$$\chi(\hat{B}^i) = \varepsilon^{ijk}\nabla_j \zeta_{Bk}$$

are those which together with the local deformations form the class τ.

The extremal conditions then read

$$\chi(\hat{s}) = 0 \qquad \chi \in \tau$$

or in more detail; the variation by local deformations give

$$\nabla_k\left(\frac{1}{T}\zeta_{ji}^{Hk}\right) = 0$$

while the variation in the other directions give

$$\nabla_i \, \partial_u \hat{s} = 0$$
$$\nabla_i \nabla_{j_k} \hat{s} + \zeta_{ie} \zeta^{km} \nabla_m \nabla_{j_l} \hat{s} = 0$$
$$\nabla_{p_{mi}} \hat{s} = 0$$
$$\nabla_{D^i} \hat{s} - \nabla_i \nabla_q \hat{s} = 0$$
$$\nabla_i \nabla_\rho \hat{s} = 0 \qquad \varepsilon^{ijk} \nabla_j \nabla_{D^k} \hat{s} = 0$$
$$\partial_{\sigma_n} \hat{s} = 0 \qquad \varepsilon^{ijk} \nabla_j \nabla_{B^k} \hat{s} = 0$$
$$\nabla_{\eta_n} \hat{s} = 0$$

Notice that the sixth condition is implied by the fourth. It is thus superfluous and will be dropped in the following.

Let β, Ω^i, ω^i, ϕ, μ, τ_n, v_n, e_i and h_i denote the intensive variables corresponding to u, j_i, p_{mi}, q, ρ, σ_n, η_n, D^i and B^i with respect to $\hat{s}$, i.e. $\beta = \partial_u \hat{s}$, $\Omega^i = \nabla_{j_i} \hat{s}$, etc. One can relate these to the intensive variables in the original coordinates in the energy representation. Thus, for example

$$\beta = \frac{1}{T}$$

$$\Omega^i = -\frac{1}{T} \sum_{n=1}^{N} \frac{\rho_n v_n^i}{\rho} \equiv -\frac{1}{T} V^i$$

$$\omega_m^i = -\frac{1}{T} \left(v_{m+1}^i - \sum_{n=1}^{m} \frac{\rho_n v_n^i}{\sum_{\alpha=1}^{m} \rho_\alpha} \right)$$

$$e_i = -\frac{1}{T} (E_i + \varepsilon_{ijk} V^j B^k)$$

$$h_i = -\frac{1}{T} (H_i - \varepsilon_{ijk} V^j D^k)$$

which are recognized as the inverse temperature, velocity of the center of mass on temperature, relative velocities between sub-systems on temperature and the electric and magnetic field strengths in the center of mass frame of reference on temperature. The expressions for ϕ, μ and v_m are combinations of chemical potentials, charge densities, mass-densities and velocities on temperature.

Before starting to look at these conditions we would like to remark that neither the derivation of the local extremal condition, nor the derivation of the global conditions has any particular frame reference. This is shown by the fact that the extremal conditions admit as solutions states that describe a system whose center of mass move with uniform velocity V^i. Thus, putting $V^i = 0$, an inspection shows that the extremal states are critical points of χ^H, i.e. χ^H is zero on the equilibrium states in the center of mass frame of reference.

6. On the construction of the gradient term in the dynamical vectorfield

Let F denote the space of the possible values for the intensive variables in the entropy representation,

$$\mathcal{F} = \{(\beta, \Omega^i, \omega^i, \phi, v, \tau_n, \nu_n, e_i, h_i) \varepsilon \cdots\}$$

and let ϕ_s denote the map

$$\begin{aligned} &\mathcal{J}_q(\mathcal{E}_s) \rightarrow \mathcal{F} \\ &(u, j_i, \ldots) \mapsto (\partial_u \hat{s}, \nabla_{j_i} \hat{s}, \ldots) \end{aligned}$$

The global extremal conditions can then be formally written

$$\begin{aligned} &\hat{\beta}_{,i} \circ \mathcal{J}_1 \phi_s = 0 \\ &(\hat{\Omega}^i_{,j} + \zeta^{ik} \zeta_{jl} \Omega^l_{,k}) \circ \mathcal{J}_1 \phi_s = 0 \\ &\hat{\omega}^i \circ \phi_s = 0 \\ &(\hat{e}_i - \hat{\phi}_{,i}) \circ \mathcal{J}_1 \phi_s = 0 \\ &\hat{v}_{,i} \circ \mathcal{J}_1 \phi_s = 0 \\ &\hat{\tau}_n \circ \phi_s = 0 \\ &\hat{\nu}_n \circ \phi_s = 0 \\ &(\hat{h}_{i,j} - \hat{h}_{j,i}) \circ \mathcal{J}_1 \phi_s = 0 \end{aligned}$$

Let $\psi : \mathcal{J}_1 \mathcal{F} \rightarrow \mathcal{M}$ denote a submersion such that

$$\begin{aligned} &\delta^{jk} \partial_{\Omega^k_{,i}} \psi^\alpha = \delta^{ik} \partial_{\Omega^k_{,j}} \psi^\alpha \\ &\partial_{e_i} \psi^\alpha = -\partial_{\phi_{,i}} \psi^\alpha \\ &\partial_{h_{i,j}} \psi^\alpha = -\partial_{h_{j,i}} \psi^\alpha \\ &\partial_{\omega^i_{,j}} \psi^\alpha = \partial_{\tau_{n,i}} \psi^\alpha = \partial_{\nu_{n,i}} \psi^\alpha = \partial_{e_{i,j}} \psi^\alpha = 0 \end{aligned}$$

for $\alpha = 1, \ldots, \dim \mathcal{M}$, and let $r : \mathcal{M} \rightarrow \mathbb{R}$. By pullback with ψ we obtain a function

$$\tilde{r} = r \circ \psi : \mathcal{J}_1 \mathcal{F} \rightarrow \mathbb{R}$$

We define a family of functions by dividing the variables of $\tilde{r}$ into two groups, i.e.

$$\tilde{r}_{(\beta, \Omega^i, \phi, v, h_i)}(\beta_{,i}, \Omega^i_{,j}, \omega^i, \phi_{,i}, v_{,i}, \tau_n, \nu_n, e_i, h_{i,j})$$

The gradient of $\tilde{r}(.)$ is by definition

$$\operatorname{grad} \tilde{r}_{(.)}(.) = \nabla_{(.)} \tilde{r}_{(.)}(.) = (-\nabla_i \partial_{\beta_{,i}} \tilde{r}, -\nabla_j \partial_{\Omega^i_{,j}} \tilde{r}, \ldots)$$

and χ^G is assumed to be given by

$$\chi^G = \operatorname{grad} \tilde{r} \circ \mathcal{J}_2 \phi_s$$

Definition. A function $\tilde{r}$ given as above and satisfying the additional conditions

(i) 'Clausius-Duhem'

$$\int_{\gamma}(\beta_{,i}\,\partial_{\beta_{,i}}\tilde{r}_{(.)}+\Omega^{i}_{,j}\,\partial_{\Omega^{i}_{,j}}\tilde{r}_{(.)}+\omega^{i}\,\partial_{\omega^{i}}\tilde{r}_{(.)}+\phi_{,i}\,\partial_{\phi_{,i}}\tilde{r}_{(.)}$$
$$+v_{,i}\,\partial_{v_{,i}}r_{(.)}+\sum_{n=1}^{N}(\tau_{n}\,\partial_{\tau_{n}}r_{(.)}+v_{n}\,\partial_{v_{n}}r_{(.)})$$
$$+e_{i}\,\partial_{e_{i}}\tilde{r}_{(.)}+h_{i,j}\,\partial_{h_{i,j}}\tilde{r}_{(.)})\circ\mathcal{J}_{2}\phi_{s}\,d^{3}x\geqslant 0$$

(ii) $\tilde{r}_{(.)}(0)=0$ and $\operatorname{grad}\tilde{r}_{(.)}(0)=0$
(iii) $\tilde{r}$ has the units entropy density on time will be called a *dissipation function.*

Theorem. *Any vectorfield χ^{G} constructed from a dissipation function in the above manner satisfies the dynamical postulate.*

Proof. By inspection. ■

The map ψ is assumed to contain the information about the dissipation mechanisms, and the function r is assumed to contain the information about the dissipation coefficients. Presumably ψ should be the same for the whole class of systems described by the same kind of observables, i.e. as for example the N-component charged fluids, while r depends on the systems particular physical and chemical properties.

To exemplify this, let $\mathcal{M}=\{(\alpha,\gamma,\delta,\varepsilon,\zeta,\theta_{m},\lambda,\tau_{n},v_{n})\}$ and let ψ be defined by

$$\alpha=\tfrac{1}{2}\delta^{ij}\delta_{kl}\Omega^{k}_{,i}(\Omega^{l}_{,j}-2\beta^{-1}\Omega^{l}\beta_{,j})$$
$$+\tfrac{1}{2}\Omega^{i}_{,j}(\Omega^{j}_{,i}-2\beta^{-1}\Omega^{j}\beta_{,i})$$
$$+\tfrac{1}{2}\delta^{ij}\delta_{k1}\beta^{-2}\Omega^{k}\Omega^{1}\beta_{,i}\beta_{,j}+\tfrac{1}{2}(\Omega^{i}\beta_{,i})^{2}$$

$$\gamma=\tfrac{1}{2}\Omega^{i2}_{,i}-\beta^{-1}\Omega^{i}\beta_{,i}\Omega^{j}_{,j}+\tfrac{1}{2}\beta^{-2}(\Omega^{i}\beta_{,i})^{2}$$

$$\delta=\tfrac{1}{2}\delta^{ij}\beta_{,i}\beta_{,j}$$

$$\lambda=\delta^{ij}(\tfrac{1}{2}v_{,i}v_{,j}-\beta^{-1}vv_{,i}\beta_{,j}+\tfrac{1}{2}\beta^{-2}v^{2}\beta_{,i}\beta_{,j})$$

$$\varepsilon=\delta^{ij}(\tfrac{1}{2}(e_{i}-\phi_{,i})(e_{j}-\phi_{,j})-\beta^{-1}\phi(e_{i}-\phi_{,i})\beta_{,j}$$
$$+\tfrac{1}{2}\beta^{-2}\phi^{2}\beta_{,i}\beta_{,j})$$

$$\zeta=\delta^{ij}\delta^{kl}(\tfrac{1}{4}(h_{i,k}-h_{k,i})(h_{j,l}-h_{l,j})$$
$$-\beta^{-1}h_{i}\beta_{,k}(h_{j,l}-h_{l,j})+\tfrac{1}{2}\beta^{-2}(h_{i}\beta_{,k}h_{j}\beta_{,l}-h_{i}\beta_{,j}h_{k}\beta_{,l}))$$

$$\theta_{m}=\tfrac{1}{2}\delta_{ij}\omega^{i}_{m}\omega^{j}_{m}$$

The components of χ^G are then given by

$$\chi^G(\hat{u}) = \nabla_i(\delta^{ij}\kappa\nabla_j T + \delta_{jk}\sigma^{ij}V^k + c_E\Phi(E_j + {}_{jkl}V^kB^l + \Phi_{,j}) + c_H\varepsilon^{ijk}\varepsilon_k^{lm}(H_j - \varepsilon_{jn0}V^nD^0)\nabla_l(H_m - \varepsilon_{mrt}V^rD^t) + c_\mu\mu\mu_{,j})$$

$$\chi^G(\hat{j}_i) = \nabla_j\sigma^{jk}\delta_{ki}$$

$$\chi^G(\hat{p}_{mi}) = \delta_{ij}\,\partial_{\theta_m}r\omega^j$$

$$\chi^G(\hat{q}) = -\nabla_i(\delta^{ij}c_E(E_j + \varepsilon_{jlm}V^lB^m + \Phi_{,j}))$$

$$\chi^G(\hat{\rho}) = \nabla_i(\delta^{ij}c_\mu\mu_{,j})$$

$$\chi^G(\hat{\sigma}_n) = \partial_{\tau_n}r$$

$$\chi^G(\hat{\eta}_n) = \partial_{v_n}r$$

$$\chi^G(\hat{D}^i) = -\varepsilon^{ij}c_E(E_j + \varepsilon_{jlm}V^lB^m + \Phi_{,j})$$

$$\chi^G(\hat{B}^i) = -\nabla_j(c_B\varepsilon^{ijk}\varepsilon_k^{lm}\nabla_l(H_m - \varepsilon_{mn0}V^nD^0))$$

where

$$\sigma^{ij} = \eta(\delta^{ik}V^j_{,k} + \delta^{jk}V^i_{,k} - \tfrac{2}{3}\delta^{ij}V^k_{,k}) + \xi\delta^{ij}V^k_{,k}$$

$$\eta = \frac{1}{T}\partial_\alpha r$$

$$\xi = \frac{1}{T}(\tfrac{2}{3}\,\partial_\alpha r + \partial_\gamma r)$$

$$\kappa = \left(\frac{1}{T}\right)^2 \partial_\delta r$$

$$c_E = \frac{1}{T}\partial_\varepsilon r$$

$$c_B = \frac{1}{T}\partial_\zeta r$$

$$c_\mu = \frac{1}{T}\partial_\lambda r$$

$$\Phi = -T\phi$$

We recognize in $\chi^G(\hat{u})$ and $\chi^G(\hat{j}_i)$ standard expressions for the dissipative part of the dynamical vectorfield of a viscous fluid [1]. This "proves" that the dissipative term in the dynamical vectorfield is a gradient vector field and that the hypotheses on which we based its construction are quite reasonable. The choice of ψ is however, a function of the result we wanted to obtain; it is possible that this choice can be improved and that one can establish ψ at least partially by means of symmetry-considerations etc.

With the above choice of $r_{(.)}$ as a family of functions on $\mathcal{M}$, the dissipation coefficients are also families of functions on $\mathcal{M}$. The procedure can be generalized by assuming that $r_{(.)}:\mathcal{J}_q(\mathcal{M})\to\mathbb{R}$. The only change this lead to in the above expressions concerns the dissipation coefficients; thus, $\eta=(1/T)\nabla_\alpha r:\mathcal{J}_q(\mathcal{M})\to\mathbb{R}$, etc.

7. Non isolation

In the preceding discussion about the dynamics we have assumed that the system is isolated. We do believe however, that the basic ideas behind the construction of the dynamical vectorfield should still be valid if this condition is abolished.

External action is simulated by 'non-conservative' boundary conditions or external electromagnetic fields. However, formally this amounts to the same thing, because one can reestablish the standard 'conservative' boundary conditions by a map that may be time dependent and induced by a space map, at the cost of introducing fictive 'external fields'.

An immediate consequence of introducing an external action is thus to 'modify' the thermodynamic potentials, either by a direct introduction of the external fields, or by the pullback with a map that reestablishes the 'conservative' boundary conditions. In either case, both the homogeneity and isotropy of space is broken, and this will show up in the thermodynamic potentials, as for example the energy-density. Thus, even if the Hamiltonian term is derived in the same way as for the isolated system, the conservation laws it satisfies in this case will no longer all be valid.

As concerns the computation of the gradient term of the dynamical vectorfield in the isolated case, it seems to be reasonable to assume that this can be done in the same way as for the isolated case, even if the second law of thermodynamics is no longer valid.

8. Appendix: Mathematical preliminaries and notations

Let $\pi:\mathcal{E}\to X$ be a fibred manifold and denote by $\mathcal{J}_q(\mathcal{E})$ the q-jet extension of $\mathcal{E}\to X$ [4]. $\mathcal{J}_q(\mathcal{E})$ is a manifold for which there exist canonical fibrations over $\mathcal{J}_r(\mathcal{E})$, π^q_r $(0<r<q)$, E, π^q_0 and X, π^0. Let (x^i), $i=1,\ldots,n$, denote local coordinates on X and (x^i, y^α), $\alpha=1,\ldots,m$, on $\mathcal{E}$. The corresponding canonical coordinates on $\mathcal{J}_q(\mathcal{E})$ are denoted by $(x^i, y^\alpha_{,\beta_\mu})$ where β_μ is a multi-index, $\beta_\mu=(0, i_1,\ldots,i_\mu)$ modulo any permutation, $i_r=1,\ldots,n$, and $\mu=0,1,\ldots,q$; $y^\alpha_{\beta_0}=y^\alpha_{,0}=y^\alpha$. The dimension $\mathcal{J}_q(\mathcal{E})$ is thus $n+m[(q+n)!/q!\,n!]$.

The canonical dual bases of the 1-form and the vectorfields on $\mathcal{J}_q(\mathcal{E})$ are denoted $(dx^i, dy^\alpha_{,\beta_\mu})$ and $(\partial x^i, \partial y^\alpha_{,\beta_\mu})$. Another interesting pair of dual bases are $(dx^i, w^\alpha_{,\beta_\mu})$ and $(\nabla_i, \partial y^\alpha_{,\beta_\mu})$, where

$$w^\alpha_{\beta_\mu}=dy^\alpha_{,\beta_\mu}-y^\alpha_{,\beta_{\mu+1}}\,dx^{i_{\mu+1}}, \qquad \mu=0,\ldots,n-1$$

and

$$\nabla_i = \partial_{x^i} + y^{\alpha}_{,\beta_{\mu+1}}\,\partial_{y^{\alpha},\beta_\mu} = \partial_{x^i} + y^{\alpha}_{,i}\,\partial_{y^\alpha} + \cdots$$
$$+ y^{\alpha}_{,ii_1\cdots i_{q-1}}\,\partial_{y^{\alpha}_{,i_1\cdots i_{q-1}}}$$

where we have assumed a generalized Einstein's summation convention.

The vectorfields χ on $\mathcal{J}_q(\mathscr{E})$ such that $w^{\alpha}_{,\beta_\mu}(\chi)=0$ are called *horizontal* vectorfields. They are 'tangent' to X, and of the form $\chi^i\nabla_i$. The vectorfields on $\mathcal{J}_q(\mathscr{E})$ of the form

$$\nabla_{i_1}\cdots\nabla_{i_\mu}\chi^\alpha\,\partial_{y^{\alpha}_{,\beta_\mu}} = \chi^\alpha\,\partial_{y^\alpha} + \nabla_i\,\partial_{y^{\alpha}_{,i}} + \cdots + \nabla_{i_1}\cdots\nabla_{i_q}\chi^\alpha\,\partial_{y^{\alpha}_{,i_1\cdots i_q}}$$

are called *vertical* vectorfields. They are "tangent" to the fibres of $\mathscr{E}\to X$.

A q-differentiable section

$$\gamma: X\to \mathscr{E},\ (x^i)\mapsto (x^i, y^\alpha(x^i))$$

can be uniquely prolonged to a section

$$j_q(\gamma): X\to \mathcal{J}_q(\mathscr{E}),\ (x^i)\mapsto (x^i, y^\alpha(x^i), \partial_{x^i}y^\alpha(x^i), \ldots, \partial_{x^{i_1}}\cdots\partial_{x^{i_q}}y^\alpha(x^i))$$

On the other hand, a section $j: X\to\mathcal{J}_q(\mathscr{E})$ is the extension of a section $\gamma: X\to\mathscr{E}$ if and only if $j_*\,\partial_{x^i} = \nabla_i\circ j_q(\gamma)$; or equivalently, $j^*w^{\alpha}_{\beta_\mu}=0$.

Let χ be any horizontal vectorfield and let $f:\mathcal{J}_q(\mathscr{E})\to\mathbb{R}$ be any function that is the pullback of a function $\mathcal{J}_r(\mathscr{E})\to\mathbb{R}$ $(0\le r<q)$ under the canonical submersion $\mathcal{J}_q(\mathscr{E})\to\mathcal{J}_r(\mathscr{E})$. We then have

$$\chi(f)\circ j_q(\gamma) = (\chi^i\nabla_i f)\circ j_q(\gamma) = \chi^i\circ j_q(\gamma)\,\partial_{x^i}f\circ j_q(\gamma)$$

This shows that ∇_i is the total derivative. Moreover, it may be considered as a linear map of functions with the property that if $f:\mathcal{J}_r(\mathscr{E})\to\mathbb{R}$ then $\nabla_i f:\mathcal{J}_{r+1}(\mathscr{E})\to\mathbb{R}$; in particular, $\nabla_i y^{\alpha}_{,\beta_\mu} = y^{\alpha}_{,\beta_\mu+1}$.

The exterior differential algebra on $\mathcal{J}(\mathscr{E})$ obviously has horizontal and vertical subalgebras. In particular, the horizontal n-forms (X-volume forms) are given by

$$\tilde f = f\frac{1}{n!}\,\varepsilon_{i_1\cdots i_n}\,dx^{i_1}\cdots dx^{i_n}$$

Let γ be a section of $\mathscr{E}\to X$; then,

$$F(\gamma) = \int_\gamma \tilde f = \int_X f\circ j_q(\gamma)\frac{1}{n!}\,\varepsilon_{i_1\cdots i_n}\,dx^{i_1}\wedge\cdots\wedge dx^{i_n} \qquad (*)$$

will be referred to as the integral of f over γ.

Let $\mathscr{B}(\mathscr{E})$ denote a set of sections $X\to\mathscr{E}$, endowed, with a differential Banach structure. A horizontal n-form $\tilde f$ then defines a function

$$F:\mathscr{B}(\mathscr{E})\to\mathbb{R}$$

by (*), provided the integral exists for all $\gamma\in\mathscr{B}(\mathscr{E})$.

The exterior differential dF of a differentiable function $F:\mathscr{B}(\mathscr{E})\to\mathbb{R}$ is a linear form on the vectorfields on $\mathscr{B}(\mathscr{E})$; i.e. $\chi \mapsto dF(\chi)$, where $dF(\chi)(\gamma)$ is the derivative in the direction χ at γ

$$dF(\chi)(\gamma) \equiv \lim_{t=0} \frac{1}{t}(F(\gamma + t\chi) - F(\gamma))$$

$$= \int_X (\partial_{y_{\beta_\mu}} f) \circ j_q(\gamma)\, \partial_{x^{i_1}} \cdots \partial_{x^{i_\mu}} \chi^\alpha \circ j_q(\gamma) \frac{1}{n!} \varepsilon_{i_1 \cdots i_n} dx^{i_1} \wedge \cdots \wedge dx^{i_0}$$

$$= \int_\gamma \chi^\alpha \nabla_{y^\alpha} f \frac{1}{n!} \varepsilon_{i_1 \cdots i_n} dx^{i_1} \wedge \cdots \wedge dx^{i_n} + \text{surface integrals}$$

where

$$\nabla_{y^\alpha} = (-1)^\mu \nabla_{i_1} \cdots \nabla_{i_\mu} \partial_{y^\alpha_{,\beta_\mu}} = \partial_{y^\alpha} - \nabla_i \partial_{y^\alpha_{,i}} + \cdots$$

A vectorfield on $\mathscr{B}(\mathscr{E})$ is a symbol and a set of boundary conditions. It will be assumed in this paper that the boundary conditions forming part of the definitions of the vectorfields on $\mathscr{B}(\mathscr{E})$ are chosen in such a way that the surface integrals vanish. Notice that the symbol for a vectorfield on $\mathscr{B}(\mathscr{E})$ "is" a vertical vectorfield on $\mathscr{J}_q(\mathscr{E})$. Part of the differential calculus on $\mathscr{B}(\mathscr{E})$ can thus be deferred to a differential calculus on the horizontal n-forms by means of differential operators of the form $\chi^\alpha \nabla_{y^\alpha}$. Thus, the integral of

$$\chi(\tilde{f}) = \chi^\alpha \nabla_{y^\alpha} f \frac{1}{n!} \varepsilon_{i_1 \cdots i_n} dx^{i_1} \wedge \cdots \wedge dx^{i_n}$$

differs from the integral of

$$d\tilde{f}(\nabla_{i_1} \cdots \nabla_{i_\mu} \chi^\alpha \partial_{y^\alpha_{,\beta_\mu}}) = \partial_{y^\alpha_{,\beta_\mu}} f \nabla_{i_1} \cdots \nabla_{i_\mu} \chi^\alpha \frac{1}{n!} \varepsilon_{i_1 \cdots i_n} dx^{i_1} \wedge \cdots \wedge dx^{i_n}$$

only by a number of partial integrations making appear vanishing surface integrals. By abuse of language we will thus say that $\chi(\tilde{f})$ is the derivative of $\tilde{f}$ in the direction χ, or write $\chi(\tilde{f}) = d\tilde{f}(\chi)$. Most of the time we will drop the volume form and write only $\chi(f)$ for $\chi^\alpha \nabla_{y^\alpha} f$ where f is a function, $\chi(f)$ is then also a function. The force of this notation lies in the fact that if a curve $c : [t_1, t_2] \to \mathscr{B}(\mathscr{E})$ is a solution of an ordinary differential equation

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

on $\mathscr{B}(\mathscr{E})$, then $\chi(f)$ measures the variation of f along c, i.e.

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

This means that a function f (or n-forms $\tilde{f}$) is a constant of motion for χ, if there exists functions ζ^i such that

$$\chi(f) = \nabla_i \zeta^i$$

To justify the above definitions of differential operators one has to show that their definitions are invariant under isomorphisms of $\mathscr{J}_q(\mathscr{E})$ induced from isomorphisms of $\mathscr{E} \to X$ of the form

$$\phi : \mathscr{E} \to \mathscr{E};\ (x^i, y^\alpha) \mapsto (x^i, \phi^\alpha(x^i, y^\alpha))$$

The isomorphism $\phi : \mathscr{E} \to \mathscr{E}$ induces an isomorphism

$$\mathscr{J}_q\phi : \mathscr{J}_q(\mathscr{E}) \to \mathscr{J}_q(\mathscr{E});\ (x^i, y^\alpha_{,\beta_\mu}) \mapsto (x^i, \nabla_{i_1} \cdots \nabla_{i_\mu}\phi^\alpha(x^i, y))$$

The canonical bases $(\partial x^i, \partial_{y^\alpha_{,\beta_\mu}})$ and $(\partial x^i, \partial_{z^\alpha_{,\beta_\mu}})$ of $T_*\mathscr{J}_{q-1}\mathscr{E}$ are related by the tangent map, i.e.

$$\begin{aligned}\partial_{z^\alpha} &= (\partial_{z^\alpha}\phi^{-1\beta}) \circ \phi\ \partial_{y^\beta} + (\partial_{z^\alpha}\nabla_i\phi^{-1\beta}) \circ \phi\ \partial_{y^\beta_{,i}} + \cdots \\ &\quad + (\partial_{z^\alpha}\nabla_{i_1} \cdots \nabla_{i_{q-1}}\phi^{-1\beta}) \circ \phi\ \partial_{y^\beta_{,i_1 \cdots i_{q-1}}} \\ &\ \ \vdots \\ \partial_{z^\alpha_{,i_1 \cdots i_{q-1}}} &= (\partial_{z^\alpha_{,i_1 \cdots i_{q-1}}}\nabla_{j_1} \cdots \nabla_{j_{q-1}}\phi^{-1\beta}) \circ \phi\ \partial_{y^\beta_{,j_1 \cdots j_{q-1}}}\end{aligned}$$

The ∇_i in the above formulae is to be considered as

$$\partial_{x^i} + z^\alpha_{,\beta_\mu+1}\ \partial_{z^\alpha_{,\beta_\mu}}$$

This notation is justified by the following proposition.

Proposition. *The local form of ∇_i is invariant under morphisms of the above class.*

Proof. The proof follows from the observation that $y^\alpha_{,\beta_\mu}$ and $z^\alpha_{,\beta_\mu}$ are related by the tangent map $T_*\mathscr{J}_{q-1}\phi$, thus, in simplified notation

$$\begin{aligned}(\partial_{x^i} + z_{,i} \cdot \partial_z) \circ \mathscr{J}_q\phi^{-1} &= \partial_{x^i} + (T_*\mathscr{J}_{q-1}\phi \cdot y)_{,i} T_*^{-1}\mathscr{J}_{q-1}\phi \cdot \partial_y \\ &= \partial_{x^i} + y_{,i} \cdot \partial_y = \nabla_i \quad \blacksquare\end{aligned}$$

Under a general isomorphism $\mathscr{J}_q(\mathscr{E}) \to \mathscr{J}_q(\mathscr{E})$ which is induced by an isomorphism $\phi : \mathscr{E} \to \mathscr{E};\ (x, y) \to (\varphi(x), \phi(x, y))$,

$$\nabla'_i \circ \mathscr{J}_q\phi = (\partial_{x^i}\varphi^j)^{-1}\nabla_j$$

Proposition. *The bases (∇_{y^α}) and (correspondingly defined) (∇_{z^α}) are related by*

$$\nabla_{z^\alpha} \circ \mathscr{J}_q\phi = (\partial_{y^\alpha}\phi^\beta)^{-1}\nabla_{y^\beta}$$

i.e. the components of $\chi = \chi^\alpha\nabla_{y^\alpha}$ transform by

$$\chi^\alpha \mapsto (\partial_{y^\beta}\phi^\alpha) \circ \phi^{-1}\chi^\beta \circ \mathscr{J}_q\phi^{-1}$$

Proof. By computation. $\blacksquare$

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