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Green formula and Legendre transformation

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Abstract. It is shown that the Legendre transformation and related hamiltonian formalism are a geometrical interpretation of the Green formula in the calculus of variations. The particular case of higher order mechanics is considered in details.

1. Introduction

It may seem paradoxal that the famous Legendre transformation appeared in numerous contexts in mathematics and theoretical physics for about 200 years is not well-understood conceptually yet. In particular, its conceptual definition is still to be found. Some long standing problems in calculus of variations and related areas of its applications are due exactly to this fact. For instance, the natural problem on what should be the Hamiltonian formalism for arbitrary order and multiplicity Lagrangians (see, e.g., [6, 18, 22, 24]) is firmly resisting a solution. Even in the most studied situations, namely, in mechanics (arbitrary order ordinary integrals) and classical field theory (first order multiple integrals) singular Lagrangians are not still understood completely in that sense (see [7, 28, 8, 12, 15, 16, 27]).

It is worth noticing that in textbooks dedicated to calculus of variations the Legendre transformation is defined (better to say, described) just by an explicit expression in terms of a local chart (e.g., [10, 11]) and only for two simplest classes of Lagrangians mentioned above. Moreover, its invariance, i.e. independence of the local chart, is not usually even mentioned. This reflects well the current mentality in the area where analytical aspects prevail traditionally all others.

A necessity to understand better the nature of the Legendre transformation arose at sixties in connection with some problems in field theory. Since then two essential steps were done in that direction. First, a manifestly invariant geometrical description of the Legendre transformation was found (see, for instance [6, 23, 13, 9, 14]) and the relative Hamiltonian field, also called K- or time evolution operator, associated with a given Lagrangian was discovered. It is worth noticing that this very important associate of the Legendre transformation was brought for the first time to the light rather recently, at 1982, in [17]. Its structure and relevance were clarified even later ([2, 4, 26, 5, 27]).

But 'invariant' does not mean 'conceptual'. So, in spite of the aforementioned progress the question "what is the Legendre transformation" is still open. In this paper we show that the answer "a suitable geometrical interpretation of the cohomological Green formula" is very plausible. Namely, we demonstrate that it is so for ordinary of arbitrary order Lagrangians. The peculiarity of this case is that for it the required geometrical interpretation can be attained on the level of finite order jets. On the contrary, in the general case a recourse to Secondary Calculus (see [32, 33]) and, as consequence, to infinite jets seems to be as inevitable as natural. These topics will be discussed in a separate paper.

The paper is organized as follows. Section 2 contains the necessary background on infinite jets: the Cartan distribution, secondary vector fields, $\mathcal{C}$-differential operators and horizontal cohomology. The main facts on the cohomological Green formula are summarized in Section 3 by starting from the linear case. Next, this formula is applied to the calculus of variations. The Legendre transformation is discussed in Section 4 as a geometric aspect of the Green formula. Then, the case of higher order mechanics is detailed. Finally, Section 5 contains, also in this particular situation, the derivation of the Hamilton canonical equations from this point of view.

2. Preliminaries on jet spaces

In this section we collect the necessary facts concerning jet spaces and differential calculus on them and fix the notation. See [20, 21, 33] for further details.

Let $Y = Y^{n+m}$ be an $(n+m)$-dimensional smooth manifold. Fix integers $m, n \geq 0$. A k-th order jet (of n-dimensional submanifolds of Y) is an equivalence class of n-dimensional submanifolds of Y which are tangent one another with the k-th order at a point of Y. Here $k = \infty$ is also admitted. The k-jet of an n-dimensional submanifold $L \subset Y$ at a point $a \in L$ is denoted by $[L]_a^k$.

The set $J^k = J^k(Y, n)$ of all k-jets of n-dimensional submanifolds of Y carries naturally a structure of a smooth manifold which is called *k-th jet manifold* (of n-dimensional submanifolds of Y).

If $L \subset Y$, $\dim L = n$, then the map

$$j_k(L) : L \longrightarrow J^k(Y, n) \quad \text{with} \quad j_k(L)(a) = [L]_a^k$$

is the *k-jet prolongation* of the imbedding $L \in Y$.

Natural projections $J^k \to J^l$, $[L]_a^k \mapsto [L]_a^l$, $k \geq l$ form the chain of maps

$$Y = J^0 \leftarrow J^1 \leftarrow \cdots \leftarrow J^k \leftarrow \cdots \leftarrow J^\infty \tag{2.1}$$

showing J^∞ to be its inverse limit.

A local chart $(y_1, \ldots, y_{m+n})$ in Y one part of which, say, $(y_{r_1}, \ldots, y_{r_n})$ is interpreted as *independent variables* $x_1 = y_{r_1}, \ldots, x_n = y_{r_n}$, while the resting part $u^1 = y_{s_1}, \ldots, u^m = y_{s_m}$ as *dependent* variables is called *divided*. Such a divided chart induces a local chart on J^k formed by functions x_j, $j = 1, \ldots, n$, and u^i_σ, $i = 1, \ldots, m$, $|\sigma| \leq k$, where $\sigma = (\sigma_1, \ldots, \sigma_n)$ is a multi-index and $|\sigma| = \sigma_1 + \cdots + \sigma_n$. Functions u^i_σ's on J^k are defined uniquely by the property:

$$u^i_\sigma \circ j_k(L) = \frac{\partial^{|\sigma|} f_i}{\partial x_\sigma},$$

for any n-dimensional submanifold $L \in Y$ represented locally in the form $L = \{u^i = f_i(x_1, \ldots, x_n),\ i = 1, \ldots, m\}$. Note that for $k = \infty$ there is no limitations on σ.

The sequence of inclusions of smooth functions algebras is associated with sequence (2.1):

$$C^\infty(J^o) \hookrightarrow C^\infty(J^1) \hookrightarrow \ldots \hookrightarrow C^\infty(J^k) \hookrightarrow \ldots \tag{2.2}$$

The direct limit of (2.2) is called the *smooth functions algebra* on J^∞. We denote it by $\mathcal{F} = \mathcal{F}(J^\infty)$ though $C^\infty(J^\infty)$ would be more expressive. Denote also by $\mathcal{F}_k = \mathcal{F}_k(J^\infty)$ the image of $C^\infty(J^k)$ in $\mathcal{F}$. This way one gets a filtration of $\mathcal{F}$:

$$\mathcal{F}_0 \subset \mathcal{F}_1 \subset \cdots \subset \mathcal{F}_k \subset \cdots \subset \mathcal{F}. \tag{2.3}$$

In terms of coordinates a smooth function f on J^∞ is a function depending on a finite number of coordinates $(x, u, \ldots, u^i_\sigma, \ldots)$.

The same procedure is applied to describe any kind of "covariant" objects on J^∞. For instance, a differential form on J^∞ may be viewed as a differential form on one of jet spaces J^k's, $k < \infty$, lifted to J^∞. Dually, a "controvariant" object on J^∞ may be understood as the inverse limit of the same kind of objects defined on finite jets along chain of maps 2.1. For instance, a tangent vector ξ to J^∞ at a point $\theta \in J^\infty$ may be viewed as a sequence $\xi_k \in T_{\theta_k} J^k$, $k = 0, 1, \ldots,$ such that $\theta_k = \pi_{\infty,k}(\theta)$ and $d_{\theta_k}\pi_{k,l}(\theta_k) = \theta_l$.

Assume now that Y is fibered $\pi : Y \to M, \quad \dim M = n$. Then one gets the k-th jet space $J^k(\pi)$, $k = 0, 1, \ldots, \infty$, of π by specifying the above construction to submanifolds of the form $L = s(M)$, $s : M \to Y$ being a (local) section of π . An *adopted* to π local chart on Y respecting the fibre structure is composed of a local chart $\{x_j\}$ on M completed by some "fibre coordinates" $\{u^i\}$. Note that $J^k(\pi)$ is an open everywhere dense domain in $J^k(Y, n)$.

A basic for the theory of PDE's geometrical structure on J^∞ is the *Cartan distribution*, or *infinite order contact structure*, $\theta \overset{\mathcal{C}}{\longmapsto} C_\theta$, $\theta \in J^\infty$, where

$$C_\theta = T_\theta(L^{(\infty)}) \quad \text{if} \quad \theta = [L]^\infty_a$$

and $L^{(\infty)}$ stands for the image of $j_\infty(L)$. Obviously, $\dim C_\theta = n$.

The Cartan distribution is generated locally by *total derivatives* $D_k = \partial/\partial x_k + \sum_{i,\sigma} u^i_{\sigma+1_k}\partial/\partial u^i_\sigma$, $1 \le k \le n$ (interpreted as vector fields on J^∞). So, it is *Frobenius, or involutive* one. It also may be viewed as the annihilator of the system of Cartan forms $\omega^i_\sigma = du^i_\sigma - \sum_k u^i_{\sigma+1_k}\, dx_k$,i.e., a vector $\xi \in T_\theta(T^\infty)$ belongs to C_θ iff on $\xi \rfloor \omega^i_\sigma = 0$ for all i, σ.

A submanifold $N \subset J^\infty$ is called *integral* (with respect to $\mathcal{C}$), if $T_\theta N = C_\theta$ for any $\theta \in N$. Locally any integral submanifold is of the form $L^{(\infty)}$ (the image of $j_\infty(L), L \subset Y$). Therefore, the set of integral submanifolds is identified with the set of immersed n-dimensional submanifolds of Y (resp., multi-valued sections of π, if $J^\infty = J^\infty(\pi)$.

Differential operators and other standard elements of differential calculus are easily constructed on J^∞ within the framework of calculus over *(filtered) commutative algebras* (see [29, 19, 25]). Namely, it means that one must deal with *filtered modules* $P = \{P_i\}$ over the filtered algebra $\mathcal{F} = \{\mathcal{F}_i\}$ (see 2.3). A *filtered differential operator*

$$\Delta : P = \{P_i\} \to Q = \{Q_j\}$$

of order $\le k$ is an $\mathbb{R}$-linear map such that

$$[f_0, [f_1, \ldots [f_k, \Delta] \ldots]] = 0, \quad \forall f_0, \ldots, f_k \in \mathcal{F}$$

where f_i's are understood as multiplication operators and $\Delta(P_i) \subset Q_{j(i)}$, $\forall i$.

In particular, vector fields on J^∞ are defined to be filtered derivations of the algebra $\mathcal{F}$. The totality of them constitutes a Lie algebra denoted by $\mathcal{D} = \mathcal{D}(J^\infty)$. Expressed in coordinates they look as

$$X = \sum_{i,\sigma} a^i_\sigma \frac{\partial}{\partial u^i_\sigma} + \sum_k b_k \frac{\partial}{\partial x_k}.$$

Summations here are infinite but it does not create any problem since smooth functions on J^∞ depend each only on a finite number of variables.

For a vector field X we write $X \in \mathcal{C}$ and say that X belongs to $\mathcal{C}$ if $X_\theta \in C_\theta$, $\forall\, \theta \in J^\infty$. The totality $\mathcal{C}D$ of all vector fields belonging to $\mathcal{C}$ is an ideal in the subalgebra

$$D_\mathcal{C} = \{X \in \mathcal{D} \mid [X, Z] \in \mathcal{D},\ \forall Z \in \mathcal{D}\}$$

of the Lie algebra $\mathcal{D}$. Obviously, $D_k \in \mathcal{C}D$.

Putting $D_\sigma = D_1^{\sigma_1} \circ \cdots \circ D_n^{\sigma_n}$ for a multi-index $\sigma = (\sigma_1, \ldots \sigma_n)$ we have

Proposition 2.1. *Any vector field $X \in D_\mathcal{C}(J^\infty)$ can be uniquely presented in the form*

$$X = \mathcal{\ni}_\varphi + \sum_k a_k D_k \tag{2.4}$$

with $\varphi = (\varphi_1, \ldots, \varphi_m)$, $\varphi_i, a_k \in \mathcal{F}(J^\infty)$ and

$$\mathcal{\ni}_\varphi = \sum_{\sigma,i} D_\sigma(\varphi_i) \frac{\partial}{\partial u^i_\sigma}.$$

The vector field $\mathcal{\ni}_\varphi$ is an *evolutionary derivation* corresponding to the *generating function* φ.

Definition 2.2. The quotient algebra

$$\varkappa = D_\mathcal{C} \big/ \mathcal{C}D$$

is called the algebra of *secondary vector fields* on J^∞.

By Proposition 2.1 $\varkappa$ is identified locally with the $\mathcal{F}$-module of generating functions Now we will distinguish an important class of differential operators on J^∞.

Definition 2.3. A differential operator $\Delta : P \to Q$ connecting two $\mathcal{F}$-modules is called *$\mathcal{C}$-differential*, if it can be restricted to any integral submanifold W of J^∞, i.e., $\Delta(p)|_W$ depends only on $p|_W$.

The totality of all $\mathcal{C}$-differential operators from P to Q is denoted by $\mathcal{C}\mathrm{Diff}(P, Q)$. It is a $\mathcal{F}$-module.

Vector fields belonging to $\mathcal{C}$, in particular, D_k's, are manifestly tangent to integral submanifolds of J^∞ and, therefore, are $\mathcal{C}$-differential. So, any matrix differential operator whose entries are of the form $\sum_\sigma a_\sigma D_\sigma$, $a_\sigma \in \mathcal{F}$ is a $\mathcal{C}$-differential one.

Proposition 2.4. *Locally all $\mathcal{C}$-differential operator is of the above form.*

Denote by $\Lambda^i(M)$ the $C^\infty(M)$-module of i-th order differential forms on a manifold M. The sequence of projections (2.1) generates the sequence of inclusions

$$\Lambda^i(J^0) \hookrightarrow \Lambda^i(J^1) \hookrightarrow \ldots \hookrightarrow \Lambda^i(J^k) \hookrightarrow \ldots$$

whose direct limit $\Lambda^i = \Lambda^i(J^\infty)$ is the $\mathcal{F}$-module of differential forms on J^∞. It is naturally filtered by images of $\Lambda^i(J^k)$'s. Local expression of a form $\rho \in \Lambda^i(J^\infty)$ looks as a finite sum

$$\rho = \sum a^{j_1\ldots j_l}_{i_1\ldots i_k\sigma_1\ldots\sigma_l} dx_{i_1} \wedge \cdots \wedge dx_{i_k} \wedge du^{j_1}_{\sigma_1} \wedge \cdots \wedge du^{j_l}_{\sigma_l}. \tag{2.5}$$

Denote by $\mathcal{C}\Lambda^i(J^\infty) \subset \Lambda^i(J^\infty)$ the $\mathcal{F}$-submodule of $\Lambda^i(J^\infty)$ composed of differential forms vanishing on the Cartan distribution $\mathcal{C}$.

Proposition 2.5. *It holds*

(i) $\mathcal{C}\Lambda^1 = \{\rho = \sum a^i_\sigma \omega^i_\sigma \mid a^i_\sigma \in \mathcal{F}\}$ *(the summation is finite),*
(ii) $\mathcal{C}\Lambda^i = \mathcal{C}\Lambda^1 \wedge \Lambda^{i-1}$*,*
(iii) $\mathcal{C}\Lambda^* = \sum \mathcal{C}\Lambda^i$ *is a differentially closed ideal in* $\Lambda^* = \sum_i \Lambda^i(J^\infty)$*.*

Remark 2.6. Exterior powers of the ideal $\mathcal{C}\Lambda^*$ are also differentially closed. They supply the de Rham complex Λ^* with a filtration. The associated spectral sequence is called the $\mathcal{C}$*-spectral sequence* and represents the natural framework in the study of cohomological aspects of PDE's and the calculus of variations (see [31, 3, 21]). In this paper we shall make use implicitly of some constructions from it.

The quotient $\bar{\Lambda}^* = \Lambda^*/\mathcal{C}\Lambda^*$ is called the algebra of *horizontal differential forms* on J^∞. The complex $\{\bar{\Lambda}^*, \bar{d}\}$, $\bar{d}$ being the quotient exterior differential, is called the *horizontal de Rham complex*. Its cohomology is the *horizontal de Rham cohomology* we denote by $\bar{H}^i$, $\bar{H}^* = \sum \bar{H}^i$.

A local expression for a horizontal form looks as

$$\omega = \sum a_{i_1,\ldots,i_q} \bar{d}x_{i_1} \wedge \cdots \wedge \bar{d}x_{i_q}, \quad a_{i_1,\ldots,i_q} \in \mathcal{F}.$$

and

$$\bar{d}\,\omega = \sum_{i_1,\ldots,i_q,k} D_k(a_{i_1,\ldots,i_q}) \bar{d}x_k \wedge \bar{d}x_{i_1} \wedge \cdots \wedge \bar{d}x_{i_q}.$$

A $\mathcal{C}$-differential operator $\square_\omega : \varkappa \to \mathcal{F}$ is associated naturally with a *Cartan form* $\omega \in \mathcal{C}\Lambda^1$:

$$\square_\omega(\varphi) := \partial_\varphi \rfloor \omega, \quad \varphi \in \varkappa.$$

Here we identify secondary vector fields with evolutionary derivations.

If $\omega = \sum a^i_\sigma \omega^i_\sigma$, $a^i_\sigma \in \mathcal{F}$, then

$$\square_\omega = (\sum_\sigma a^1_\sigma D_\sigma, \ldots, \sum_\sigma a^m_\sigma D_\sigma).$$

This row differential operator acts naturally on columns $\varphi = (\varphi_1, \ldots, \varphi_m)^T$.

Proposition 2.7. *The correspondence* $\omega \mapsto \square_\omega$ *establishes a natural isomorphism of* $\mathcal{F}$*-modules* $\eta : \mathcal{C}\Lambda^1(J^\infty) \to \mathcal{C}\mathrm{Diff}(\varkappa, \mathcal{F})$*.*

The canonical isomorphism

$$\mathcal{C}\mathrm{Diff}(\varkappa, \mathcal{F}) \otimes_\mathcal{F} \bar{\Lambda}^i \to \mathcal{C}\mathrm{Diff}(\varkappa, \bar{\Lambda}^i)$$

allows to extend naturally η to an isomorphism (still denoted η)

$$\eta : \mathcal{C}\Lambda^1 \otimes_\mathcal{F} \bar{\Lambda}^i \to \mathcal{C}\mathrm{Diff}(\varkappa, \bar{\Lambda}^i). \tag{2.6}$$

In this paper we shall use the short $X(\omega)$ for the Lie derivative of a differential form ω along a vector field X instead of the common $L_X(\omega)$. Observe also that evolutionary vector fields leave invariant the ideal $\mathcal{C}\Lambda^*$ so that they acts as quotient Lie derivatives on horizontal forms. We still denote such a quotient derivative as $\partial_\varphi(\rho),\ \rho \in \bar{\Lambda}^*$.

3. Cohomological Green's formula

The *cohomological Green's formula*, i.e., a cohomological interpretation of the classical one, was proposed by the second author in [30] (see also [31]). This formula is key for what follows. In this section a short account of main facts about we shall need further is given. For a more conceptual exposition see [21, 3].

3.1. **Adjoint operators.** In this subsection, M stands for an n-dimensional smooth manifold, $A = C^\infty(M)$, $\Lambda^k = \Lambda^k(M)$. All the tensor products are taken over A. Given A-modules P and Q a *differential operator*

$$\Delta : P \to Q$$

of order $\leq k$ is an $\mathbb{R}$-linear map such that

$$[a_0, [a_1, \ldots [a_k, \Delta] \ldots]] = 0, \quad \forall a_0, \ldots, a_k \in A.$$

In this relation a_i's are understood to be multiplication operators.

All differential operators from P to Q of order $\leq k$ constitute a left A-module denoted by $\mathrm{Diff}_k(P, Q)$. The following (left) A-modules will be of our interest further on:

$$\mathrm{Diff}(P, Q) \stackrel{def}{=} \bigcup_{k \geq 0} \mathrm{Diff}_k(P, Q),$$

$$\mathrm{Diff}_k(P) \stackrel{def}{=} \mathrm{Diff}_k(A, P), \quad \mathrm{Diff}(P) \stackrel{def}{=} \mathrm{Diff}(A, P).$$

The algebra of scalar differential operators $\mathrm{Diff}\,A$ acts on Λ^n transforming it into a right $\mathrm{Diff}\,A$-module. This action is such that for any $a \in A, X \in \mathcal{D}(M)$ and $\eta \in \Lambda^n$

$$\eta \cdot a \stackrel{def}{=} a\eta, \quad \eta \cdot D \stackrel{def}{=} -D(\eta).$$

The action is defined uniquely by these properties.

Let $\Delta \in \mathrm{Diff}\,\Lambda^n$ and $\eta \in \Lambda^n$ be a (local) volume form. Define the operator $\Delta_\eta \in \mathrm{Diff}\,A$ by $\Delta(a) = \Delta_\eta(a)\eta$. The *adjoint* to Δ operator $\Delta^* \in \mathrm{Diff}\,\Lambda^n$ is defined in terms of the aforementioned right action as

$$\Delta^*(a) = (a\eta) \cdot \Delta_\eta$$

.

Let $(x_1, x_2, \ldots, x_n)$ be a local chart, $\eta = dx_1 \wedge \cdots \wedge dx_n$ and $\Delta_\eta = \sum_\alpha a_\alpha \frac{\partial^{|\alpha|}}{\partial x^\alpha}$ where $\alpha = (\alpha_1, \ldots, \alpha_n)$ is a multi-indice. Then

$$\Delta^*(a) = \sum_\alpha (-1)^{|\alpha|} \frac{\partial^{|\alpha|}(a a_\alpha)}{\partial x^\alpha} \eta.$$

For a given A-module R put $\widehat{R} = \mathrm{Hom}_A(R, \Lambda^n)$ and associate with an element $r \in R$ the operator $o_r \in \mathrm{Diff}_0 R,\ o_r(a) = ar$. Note that $R \subset \widehat{\widehat{R}}$. Consider then an operator

$\Delta \in \mathrm{Diff}(P,Q)$, P,Q being A-modules, and associate with a couple $(p,\widehat{q})$, $p \in P$, $\widehat{q} \in \widehat{Q}$, the operator

$$\Delta(p,\widehat{q}) = o_{\widehat{q}} \circ \Delta \circ o_p \in \mathrm{Diff}\,\Lambda^n.$$

Obviously, Δ is determined completely by the family of operators $\Delta(p,\widehat{q})$. This allows to define the *adjoint* to Δ operator $\Delta^* \in \mathrm{Diff}(\widehat{P},\widehat{Q})$ by putting

$$\Delta(p,\widehat{q})^* = \Delta^*(\widehat{q},p), \quad \forall p \in P,\ \widehat{q} \in \widehat{Q}.$$

The so-defined *-operation possesses the usual properties:

$$\Delta^{**} = \Delta, \quad (\Delta \circ \Box)^* = \Box^* \circ \Delta^*,$$

for any $\Delta \in \mathrm{Diff}(P,Q)$ and $\Box \in \mathrm{Diff}(Q,R)$, etc.

3.2. **Linear Green's formula.** The following lemma is key for the Green formula.

Lemma 3.1. *There exists a differential operator*

$$ж\colon \mathrm{Diff}_k\Lambda^n \to \Lambda^{n-1}$$

of order $\leq k-1$ *such that for any* $\Box \in \mathrm{Diff}_k\Lambda^n$ *the relation*

$$\Box(1) = \Box^*(1) + d\,ж(\Box) \tag{3.1}$$

holds.

Remark 3.2. The operator ж is constructed naturally with help of a linear connection on M (see [1]). In the cases $k=1$ or $\dim M = 1$ ж is defined uniquely.

A possible local choice of the operator ж is as follows. Let the local chart, volume form η and the operators Δ and Δ_η be as in the preceding subsection. For a multi-index $\alpha = (\alpha_1,\ldots,\alpha_n)$ put

$$\alpha - 1_j = (\alpha_1,\ldots,\alpha_j - 1,\ldots,\alpha_n), \quad \eta_j = \frac{\partial}{\partial x_j}\rfloor\eta.$$

Note that a "full parallelism connection" is associated with a local chart. Then the corresponding to it operator ж (see the above remark) looks as

$$ж(\Delta) = -\sum_{|\alpha|\geq 1}\sum_{j=1}^{n}(-1)^{|\alpha|}\,\frac{\alpha_j}{|\alpha|}\,\frac{\partial^{|\alpha|-1}(a_\alpha)}{\partial x^{\alpha-1_j}}\,\eta_j \tag{3.2}$$

Let now $\Delta \in \mathrm{Diff}(P,Q)$ be a general operator. By applying Lemma 3.1 to the operator $\Box = \Delta(p,\widehat{q})$ one gets

$$\Delta(p,\widehat{q})(1) = \Delta(p,\widehat{q})^*(1) + d\,ж(\Delta(p,\widehat{q})) \tag{3.3}$$

Introducing the notation $\langle\,,\,\rangle$ natural pairings $P \otimes \widehat{P} \to \Lambda^n$, $Q \otimes \widehat{Q} \to \Lambda^n$ we see that $\Delta(p,\widehat{q})(1) = \langle\Delta(p),\widehat{q}\rangle$ and $\Delta(p,\widehat{q})^*(1) = \langle p,\Delta^*(\widehat{q})\rangle$. So, rewriting 3.3 we get the linear Green's formula.

Theorem 3.3. *For each* $\Delta \in \mathrm{Diff}_k(P,Q)$, $p \in P$, $\widehat{q} \in \widehat{Q}$, *the following relation holds*

$$\langle\Delta(p),\widehat{q}\rangle = \langle p,\Delta^*(\widehat{q})\rangle + d\,ж(\Delta(p,\widehat{q})). \tag{3.4}$$

3.3. **Green's formula in $\mathcal{C}$-theory.** Notions and results discussed previously can be extended to the "$\mathcal{C}$-*theory*" rather directly, just by putting through the substitutions:

$$\mathcal{F} \mapsto A, \quad \mathcal{C}\mathrm{Diff}_k \mapsto \mathrm{Diff}_k, \quad \bar{\Lambda}^i \mapsto \Lambda^i, \quad \bar{d} \mapsto d, \quad D^\alpha \mapsto \frac{\partial^{|\alpha|}}{\partial x^\alpha}, \quad \ldots$$

For instance, in the "$\mathcal{C}$-situation" $\widehat{R}$ means $\mathrm{Hom}_{\mathcal{F}}(R, \bar{\Lambda}^n)$ for a $\mathcal{F}$-module R, etc.

The $\mathcal{C}$-versions of Lemma 3.1 and Theorem 3.3 are summed up as

Theorem 3.4. *There is a $\mathcal{C}$-differential operator of order $\leq k-1$*

$$\text{ж}\colon \mathcal{C}\mathrm{Diff}_k\bar{\Lambda}^n \to \bar{\Lambda}^{n-1}$$

such that, for any $\Delta \in \mathcal{C}\mathrm{Diff}_k(P, Q)$, $p \in P$ and $\widehat{q} \in \widehat{Q}$ the relation

$$\langle \Delta(p), \widehat{q} \rangle = \langle p, \Delta^*(\widehat{q}) \rangle + d\,\text{ж}(\Delta(p, \widehat{q})) \tag{3.5}$$

holds.

In a local jet-chart (x_j, u^i_σ) the description of what was discussed above is as follows. We start from the *horizontal* volume form $\eta = \bar{d}x_1 \wedge \cdots \wedge \bar{d}x_n \in \bar{\Lambda}^n$. Then an operator $\Delta \in \mathcal{C}\mathrm{Diff}\ \bar{\Lambda}^n$ is described as

$$\Delta(f) = \Delta_\eta(f)\eta, \qquad \Delta_\eta = \sum_\alpha a_\alpha D^\alpha, \quad f, a_\alpha \in \mathcal{F}.$$

The corresponding description for the adjoint operator $\Delta^* \in \mathcal{C}\mathrm{Diff}_k\bar{\Lambda}^n$ is

$$\Delta^*(f) = \Delta^*_\eta(f)\eta, \quad \Delta^*_\eta = \sum_\alpha (-1)^{|\alpha|} D^\alpha \circ a_\sigma.$$

Similarly, the $\mathcal{C}$-analogue of formula 3.2 is

$$\text{ж}(\Delta) = -\sum_{|\alpha|\geq 1}\sum_{j=1}^{n} (-1)^{|\alpha|}\,\frac{\alpha_j}{|\alpha|}\,D^{\alpha - 1_j}(a_\alpha)\,\eta_j. \tag{3.6}$$

In the case $n = 1$ there exists a canonical choice of the operator ж which coincides locally with 3.6. In this case this expression becomes particularly simple. In fact, by putting $t = x_1$ we have

$$\eta = \bar{d}t, \quad \Delta(a) = \Delta_\eta(a)\eta, \quad \Delta_\eta = \sum_s a_s D^s_t$$

with D_t being the total derivative with respect to t and

$$\text{ж}(\Delta) = -\sum_{s\geq 1} (-1)^s\, D^{s-1}_t \circ a_s \tag{3.7}$$

3.4. **Green's formula in the calculus of variations.** This formula is obtained from the previous one by specializing it to the universal linearization operator corresponding to the variational functional in question.

Let $\rho \in \bar{\Lambda}^*$. The operator

$$\ell_\rho\colon \varkappa \to \bar{\Lambda}^*, \quad \ell_\rho(\varphi) = \mathcal{Э}_\varphi(\rho), \quad \varphi \in \varkappa,$$

is called the *universal linearization operator* of ρ. It should be stressed that $\ell_\omega \in \mathcal{C}\mathrm{Diff}(\varkappa, \bar{\Lambda}^n)$.

Let $\varphi \in \varkappa$ and $\omega \in \bar{\Lambda}^n$ a lagrangian density. The velocity of change of ω under the "evolution" $\mathcal{Э}_\varphi$ is described by the Lie derivative

$$\mathcal{Э}_\varphi(\omega) = \ell_\omega(\varphi) = \langle \ell_\omega(\varphi), 1\rangle \tag{3.8}$$

The Green formula (3.5) applied to ℓ_ω says

$$\ell_\omega(\varphi) = \langle \ell_\omega(\varphi), 1\rangle = \langle \varphi, \ell^*_\omega(1)\rangle + \bar{d}ж(\ell_\omega(\varphi, 1)). \tag{3.9}$$

Formula 3.9 tells that horizontal forms $\ell_\omega(\varphi)$ and $\langle \varphi, \ell^*_\omega(1)\rangle$ represent the same horizontal cohomology class. Note also that $\ell^*_\omega(1) \in \widehat{\varkappa}$.

Formula 3.9 is a "conceptual" version of the classical formula for the first variation. Its principal advantage is that it shows manifestly the mathematical nature of composing it terms. For instance, the Euler-Lagrange equation for the functional $\int \omega$ reads in these terms as

$$\ell^*_\omega(1) = 0. \tag{3.10}$$

In other words, the *Euler operator* associating with a functional the corresponding Euler-Lagrange equation looks as

$$\mathcal{E} \colon \omega \mapsto \mathcal{E}(\omega) \stackrel{def}{=} \ell^*_\omega(1).$$

Remark 3.5. It is worth stressing that the Euler operator is not $\mathcal{C}$-differential. In Secondary Calculus $\mathcal{C}$-differential operators represent zero order *secondary differential operators* while the Euler operator represents the first order one.

4. The Legendre transformation

Now we pass to analyze the second term in the right side of Green's formula 3.9. First, note that the map

$$ж_\omega \colon \varphi \longmapsto ж_\omega(\varphi) \stackrel{def}{=} ж\left((\ell_\omega(\varphi, 1)\right) \tag{4.1}$$

is a $\mathcal{C}$-differential operator. In the sequel it plays a central role.

Definition 4.1. The operator $ж_\omega \in \mathcal{C}\mathrm{Diff}(\varkappa, \bar{\Lambda}^{n-1})$ is called the *Legendre operator* associated to the lagrangian ω.

The operator $ж_\omega$ is defined up to the addend of the form $\bar{d}\circ\square$ with $\square \in \mathcal{C}\mathrm{Diff}(\varkappa, \bar{\Lambda}^{n-2})$. This arbitrariness can be eliminated only for $n = 1$ or $k = 1$.

Let $\omega = L\eta$, $L \in \mathcal{F}$, and $\eta = \bar{d}x_1 \wedge \cdots \wedge \bar{d}x_n$. In order to obtain a local expression for $ж_\omega$ we first observe that $\ell_\omega(\varphi, 1) = \mathcal{Э}_\varphi(\omega) = (\sum_\alpha a_\alpha D^\alpha)\eta$ with

$$a_\alpha = \sum_{\beta,i} \binom{\alpha+\beta}{\alpha} \frac{\partial L}{\partial u^i_\alpha} D^\beta(\varphi_i).$$

So, with the choice made in (3.6) one gets

$$ж_\omega(\varphi) = -\sum_{\alpha,j} (-1)^{|\alpha|} \binom{\alpha+\beta}{\alpha} \frac{\alpha_j}{|\alpha|} D^{\alpha-1_j} \left(\sum_{\beta,i} \frac{\partial L}{\partial u^i_{\alpha+\beta}} D^\beta(\varphi_i) \right) \eta_j \tag{4.2}$$

The isomorphism η (Proposition 2.7 and (2.6)) applied to $ж_\omega$ proves existence of a Cartan form $\Theta \in \mathcal{C}\Lambda^1 \otimes_{\mathcal{F}} \bar{\Lambda}^{n-1}$ such that

$$ж_\omega(\varphi) = \varphi \rfloor \Theta \tag{4.3}$$

The form Θ will be called the *Legendre form associated to ω*.

4.1. **What is the Legendre transformation?** Now we are going to establish a relation between the Legendre operator defined above and the Legendre transformation. In the simplest case $n = k = 1$, which covers, in particular, Lagrangian mechanics, formulae (4.2) and (4.3) looks, when passing to the notation $x_1 = t$, $u = q$, $\frac{du}{dx_1} = \dot{q}$, $\omega = L(t, q, \dot{q})dt$, etc, as

$$ж_\omega = \frac{\partial L}{\partial \dot{q}} \quad \text{and} \quad \Theta = \frac{\partial L}{\partial \dot{q}}(dq - \dot{q}dt).$$

This shows that in this case the Legendre operator and Legendre transformation coincide at least on the level of local expressions. This observation is key in revealing the nature of the Legendre transformation. In fact, the original "descriptive" definition $p = \frac{\partial L}{\partial \dot{q}}$ (even interpreted invariantly in terms of geometry of tangent and cotangent bundles) does not give reasonable indications on how to generalize it to arbitrary functionals (Lagrangians). On the other hand, since the Legendre operator is defined *naturally* for arbitrary functionals it is natural as well to conjecture that

> *in the general case the Legendre transformation is represented by the Legendre operator.*

However, this can not be taken yet as a rigorous formal definition by the following reasons. First, the density of a functional is defined only up to a full divergence term and, second, for a given density the associated Legendre operator is not unique as well. So, it is not straightforward to understand what are the domain and the range of the Legendre transformation represented by a Legendre operator. The nature of this non-uniqueness indicates unambiguously a cohomological nature of the Legendre transformation. It is worth noticing in this connection that numerous tentatives to define the Legendre transformation for general functionals in terms of local differential geometry resulted successful only for situations when this non-uniqueness can be naturally eliminated (see [6]). 'Higher order mechanics', i.e., $n = 1$ and k is arbitrary, is, maybe, most important of them. In the rest of this paper it will be shown that for 'higher order mechanics' the above conjecture is pretty confirmed by deducing from it all known in that concern results. We chose this particular case for two reasons. One of them is to illustrate the conjecture on a well established material which does not require a recourse to elements of Secondary Calculus. On the other hands, elaborating details in this relatively simple situation we get additional useful hints to face the problem in full generality.

4.2. **Legendre transformation in higher order mechanics.** For our purposes it will be sufficient to limit our considerations to the trivial bundle $\pi\colon M \times \mathbb{R} \to \mathbb{R}$, M being an m-dimensional smooth manifold. Denote by t the canonical coordinate in $\mathbb{R}$ and by $(q^1, \dots, q^m)$ a local chart on M. Then the associated chart in $J^k\pi$ (see Section 2) is (t, q_i^j), $i = 0, 1, \dots, k$, $j = 1, \dots, m$. Sometimes it will be convenient to use the short notation $q = q_0 = (q^1, \dots, q^m)$ and $q_i = (q_i^1, \dots, q_i^m)$.

Fix a k-order Lagrangian density $\omega = Ldt$, i.e., $L \in \mathcal{C}^\infty(J^k\pi)$. In this notation e:legendre becomes

$$\text{(4.4)}\qquad ж_\omega(\varphi) = -\sum_{l\geq 1}(-1)^l D_t^{l-1}\left(\sum_{r,i}\frac{\partial L}{\partial q^i_{l+r}}\binom{l+r}{r}D_t^r(\varphi_i)\right) = \sum_{i,s,r}(-1)^s D_t^s\left(\frac{\partial L}{\partial q^i_{r+s+1}}\right)D_t^r(\varphi_i)$$

or, alternatively,

$$\text{(4.5)}\qquad ж_\omega(\varphi) = \sum_{i,r} A_i^r D_t^r(\varphi_i) = (ж^1_\omega, \dots, ж^m_\omega)(\varphi_1, \dots, \varphi_m)^T$$

where

$$ж^i_\omega = \sum_r A_i^r D_t^r, \quad i = 1, \dots, m$$

if

$$A_i^r = \sum_s (-1)^s D_t^s\left(\frac{\partial L}{\partial q^i_{r+s+1}}\right)$$

In other words, in shortened notation

$$\text{(4.6)}\qquad ж_\omega = A + A^1 D_t + A^2 D_t^2 + \dots + A^{k-1}D^{k-1}$$

where the coefficients A^r are determined recurrently as

$$\text{(4.7)}\qquad \begin{cases} A^{k-1} & = L_{q_k} \\ A^{k-2} & = L_{q_{k-1}} - D_t A^{k-1} \\ \dots & \quad \dots \\ A^2 & = L_{q_3} - D_t A^3 \\ A^1 & = L_{q_2} - D_t A^2 \\ A^0 & = L_{q_1} - D_t A^1 \end{cases}$$

(here L_{q_r} stands for the row of partial derivatives $\frac{\partial L}{\partial q_r} = (\frac{\partial L}{\partial q_r^1}, \dots, \frac{\partial L}{\partial q_r^m})$).

Remark 4.2. From these relations it results that A^r depends on derivatives of order $\leq 2k - r - 1$, i.e., lies on $J^{2k-r-1}\pi$.

In view of (4.7) the Euler-Lagrange equation may be rewritten as follows. According to (3.10) we have

$$\mathcal{E}(\omega) = \ell^*_\omega(1) = \sum_r (-1)^r D_t^r(L_{q_r})\bar{d}t = (L_q - D_t A)\bar{d}t.$$

So, the Euler-Lagrange equation takes the form

$$\text{(4.8)}\qquad L_q - D_t A = 0$$

Accordingly, the Legendre form Θ (in the considered case it belongs to $\mathcal{C}\Lambda^1$) has the local expression

$$\text{(4.9)}\qquad \Theta = A^0(dq - q_1 dt) + A^1(dq_1 - q_2 dt) + \cdots A^{k-1}(dq_{k-1} - q_k dt)$$

The coefficients of Θ are functions on $J^{2k-1}\pi$ and, hence, Θ may be viewed as a form on $J^{2k-1}\pi$. The peculiarity of Θ is that for any $z \in J^{2k-1}\pi$ the co-vector

$$\Theta_z = a_0(dq - b_0 dt) + a_1(dq_1 - b_1) + \cdots + a_{k-1}(dq_{k-1} - b_{k-1}),$$

with $a_i = A^i(z)$, $b_i = q_i(z)$ may be viewed also a co-vector on J^{k-1} at the point $w = \pi_{2k-1,k-1}(z)$ vanishing on the 1-dimensional subspace

$$l_z = \{\xi \in T_w(J^{k-1}\pi) \mid \xi \rfloor (dq_i - b_i dt) = 0,\ i = 0, 1, \ldots, r-1\}$$

which is complementary to the subspace $V_w \subset T_w(J^{k-1}\pi)$ of vertical (with respect to the projection $J^{k-1}\pi \to \mathbb{R}$) tangent vectors. By this reasons Θ_z is interpreted naturally as a linear functional on V_w, i.e., as an element, denote it by Θ_z^V, of V_w^*, without any loss of information.

Definition 4.3. The correspondence

$$J^{2k-1} \ni z \stackrel{\mathcal{L}}{\longmapsto} \Theta_z^V \in V_w^*$$

is called the *Legendre map (transformation)* associated with the Lagrangian density ω.

Denote by $VJ^r\pi \to J^r\pi$ the bundle of vertical (with respect to $J^r\pi \to \mathbb{R}$) tangent to $J^r\pi$ vectors and by $V^*J^r\pi \to J^r\pi$ the dual bundle. So, the Legendre map is designed as

$$J^{2k-1}\pi \stackrel{\mathcal{L}}{\longrightarrow} V^*J^{k-1}\pi\ . \tag{4.10}$$

Remark 4.4. So, the Legendre transformation is just a suitable geometrical interpretation of the form Θ and, therefore, of the Legendre operator $ж_\omega$. It can be done, however, directly, i.e., in terms of $ж_\omega$ itself, by applying the "permutability law" $VJ^r = J^rV$. We have chosen 'forms' instead of 'operators' in order to facilitate a comparison with the standard approach.

The jet bundle $J^r\pi \to \mathbb{R}$ inherits the triviality of π and may be seen as

$$M_1^r \times \mathbb{R} \longrightarrow \mathbb{R} \tag{4.11}$$

where $M_1^r = J_0^r(\mathbb{R}, M)$ is the $(1, r)$-velocities space of M.

It is straightforwardly from (4.11) that

$$V^*J^{k-1}\pi \simeq T^*M_1^{k-1} \times \mathbb{R}. \tag{4.12}$$

This shows the range of the Legendre map to be a family of symplectic manifolds indicating directly on existence of a Poisson bracket on it.

To get a convenient local description of the Legendre map consider a jet-chart $(q, q_1, \ldots, q_{k-1})$ on M_1^{k-1} and then the associated symplectic chart $(q, q_1, \ldots, q_{k-1}, p, p^1, \ldots, p^{k-1})$ on

$T^*M_1^{k-1}$. This way one gets the chart $(t, q, q_1, \dots, q_{k-1}, p, p^1, \dots, p^{k-1})$ on $J^{k-1}\pi$. In its terms the Legendre map is, obviously, described as

$$\begin{cases} \mathcal{L}^*(t) &= t \\ \mathcal{L}^*(q_i) &= q_i, \\ \mathcal{L}^*(p^i) &= A^i, \quad i = 0, \dots k-1 \end{cases} \tag{4.13}$$

Proposition 4.5. *The Legendre map is a local diffeomorphism if and only if the Hessian matrix* $(L_{q_k q_k})$ *of the Lagrangian function* $L = L(t, q, q_1, \dots, q_k)$ *with respect to the higher order derivative coordinates is nondegenerate:*

$$\det (L_{q_k q_k}) \neq 0.$$

Proof. Observe that local expressions (4.9) can be rewritten in the form

$$\begin{cases} A^{k-1} &= L_{q_k} \\ A^{k-2} &= \phi_{k-2}(t, q, \dots, q_k) - q_{k+1}L_{q_k q_k} \\ A^{k-3} &= \phi_{k-3}(t, q, \dots, q_{k+1}) - q_{k+2}L_{q_k q_k} \\ & \dots \\ A^1 &= \phi_1(t, q, \dots, q_{2k-3}) - q_{2k-2}L_{q_k q_k} \\ A &= \phi_0(t, q, \dots, q_{2k-2}) - q_{2k-1}L_{q_k q_k} \end{cases} \tag{4.14}$$

for some functions $\phi_0, \dots, \phi_{k-2}$.

Now it is easily seen from (4.14) and (4.13) that the determinant of the Jacobian matrix of $\mathcal{L}$ is, up to a sign, the k-th power of $\det(L_{q_k q_k})$. □

5. Energy and Hamiltonian canonical equations

The energy of a Lagrangian system is the Noether current corresponding to the 'translation in time'. Compute with this purpose $\frac{\partial}{\partial t}(\omega)$ having in mind that (see decomposition (2.4))

$$\frac{\partial}{\partial t} = -\mathcal{Э}_{\dot q} + D_t \tag{5.1}$$

where we use $\dot q$ instead of q_1 as it is standard in mechanics. Then, applying the Green's formula 3.9 to $\mathcal{Э}_{\dot q}(\omega) = \ell_\omega(\dot q)$ we see that

$$\begin{aligned} \frac{\partial}{\partial t}(\omega) &= -\langle \dot q, \ell^*_\omega(1)\rangle + \bar d(-\text{ж}_\omega(\dot q) + D_t \rfloor \omega) \\ &= -\langle \dot q, \ell^*_\omega(1)\rangle + D_t(-\text{ж}_\omega(\dot q) + L)dt \end{aligned}$$

So, if ω is time-indepent, i.e., $\frac{\partial}{\partial t}(\omega) = 0$, then

$$D_t(\text{ж}_\omega(\dot q) - L) = 0 \tag{5.2}$$

on the extremals of the corresponding variational problem, i.e., solutions of the Euler-Lagrange equation $\mathcal{E}(\omega) = 0$.

Definition 5.1. The function

$$E = ж_\omega(\dot q) - L$$

is called the *energy* for the Lagrangian system associated with the Lagrangian density ω.

Hence, $E\bar{d}t$ is the *Noether current* corresponding to $\frac{\partial}{\partial t}$.

The local expression for the energy function is obtained immediately from (4.6):

$$E = q_1 \cdot A + q_2 \cdot A^1 + \cdots + q_k \cdot A^{k-1} - L \tag{5.3}$$

where we write $q_1 \cdot A$ for $q_1^1 A_1 + q_1^2 A_2 + \cdots + q_1^m A_m$, etc.

Since $A^i - L_{q_{i+1}} = -D_t(A^{i+1})$ (see (4.9)) the differential of E takes the form

$$\begin{aligned} dE =& - L_t dt - L_q dq \\ & - D_t(A^1)dq_1 - D_t(A^2)dq_2 - \cdots - D_t(A^{k-1})dq_{k-1} \\ & + q_1 dA + q_2 dA^1 + \cdots + q_k dA^{k-1} \end{aligned} \tag{5.4}$$

In view of (4.8) we obtain a new version of the Euler-Lagrange equation by substituting $D_t A$ for L_q in identity (5.4):

Proposition 5.2. *The Euler-Lagrange equation is equivalent to the relation*

$$\begin{aligned} dE =& - L_t dt - D_t(A)dq - D_t(A^1)dq_1 - \cdots - D_t(A^{k-1})dq_{k-1} \\ & + q_1 dA + q_2 dA^1 + \cdots + q_k dA^{k-1}. \end{aligned}$$

A Lagrangian density is called *regular* if the corresponding Legendre map is a diffeomorphism on its image. The following is standard:

Definition 5.3. If a density ω is regular, then the function

$$H \overset{\text{def}}{=} (\mathcal{L}^{-1})^* E \in \mathcal{C}^\infty(V^* J^{k-1}\pi)$$

is called the *Hamiltonian function* corresponding to ω.

By applying now $(\mathcal{L}^{-1})^*$ to (5.4) and using (4.13) one finds that

$$\begin{aligned} dH =& (\mathcal{L}^{-1})^* dE = -(\mathcal{L}^{-1})^* L_t dt \\ & - \bar{D}_t^{\mathcal{L}}(p)dq - \bar{D}_t^{\mathcal{L}}(p^1)dq_1 - \cdots - \bar{D}_t^{\mathcal{L}}(p^{k-1})dq_{k-1} \\ & + \bar{D}_t^{\mathcal{L}}(q)dp + \bar{D}_t^{\mathcal{L}}(q_1)dp^1 + \cdots + \bar{D}_t^{\mathcal{L}}(q_{k-1})dp^{k-1} \end{aligned} \tag{5.5}$$

where $\bar{D}_t^{\mathcal{L}} = (\mathcal{L}^{-1})^* \circ D_t \circ \mathcal{L}^*$.

In view of Proposition 5.2 the Euler-Lagrange equation for ω is equivalent to (5.5). Rewritten in terms of coefficients of figuring in it differential forms (5.5) reads as:

Proposition 5.4 (**Canonical equations**)**.** *If the Legendre map $\mathcal{L}$ is a diffeomorphism, the Euler-Lagrange equations are equivalent to the system*

$$(5.6) \qquad \frac{\partial H}{\partial t} = (\mathcal{L}^{-1})^* \frac{\partial L}{\partial t}, \qquad \begin{cases} \dfrac{\partial H}{\partial q_i} & = -\bar{D}_t^{\mathcal{L}}(p^i) \\ \dfrac{\partial H}{\partial p^i} & = \bar{D}_t^{\mathcal{L}}(q_i), \end{cases} \qquad i = 0, 1, \ldots, k-1.$$

where $q_0 = q$, $p^0 = p$.

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