BOUNDARY VALUES AS HAMILTONIAN VARIABLES: NEW POISSON BRACKETS

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Abstract

The ordinary Poisson brackets in field theory do not fulfil the Jacobi identity if boundary values are not reasonably fixed by special boundary conditions. We show that these brackets can be modified by adding some surface terms to avoid this restriction. Our definition of Poisson brackets permits to treat boundary values of a field on equal footing with its internal values and directly estimate the brackets between both surface and volume integrals. This construction is applicable to any local form of Poisson brackets. A prescription for δ-function on closed domains and a definition of the *full* variational derivative are proposed. as an example.

1 Introduction

The standard field theory Hamiltonian formalism implies that all boundary terms, arising as a result of integration by parts, are really zero. This requirement is usually fulfilled due to conditions of periodicity or rapid decay of variables at infinity [1]. But in some physical problems these conditions do not take place (for example, massless fields are slowly decaying at infinity [2]). Also there is an important class of free boundary problems (surface waves in fluids [3], [4], free motion of string ends, and so on) which requires changes in the standard approach.

Revising Hamiltonian methods to include treatment of these classes of problems it is necessary to reject the usual handling of divergencies as irrelevant terms and to incorporate them into the formalism. Therefore, both the Hamiltonian and the Poisson bracket (Hamiltonian operator) must no more be defined "up to divergencies" or "modulo divergencies".

The standard Hamiltonian approach to evolution problems or the so-called "formal variational calculus" [5] operates with a concept of local functional, defined also "modulo divergencies". We show that this restriction can be lifted and another definition of local functional can be taken as a primary concept. Local means here having integrand dependent only on field variables and their derivatives of finite order in the same point.

Further, a natural generalization of the Euler-Lagrange derivative is a full variational derivative. It is constructed as a distribution with the help of the characteristic function of a domain (or Heaviside step function) and a finite number of its derivatives. Such a full variational derivative gives the full variation of the local functional without any assumptions of zero variations on the boundary.

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The formal substitution in the Poisson brackets of these full variational derivatives instead of the Euler-Lagrange ones leads to an indefinite expression containing product of distributions. Nevertheless, as luck would have it, there are "rules of the game" with nonassociative but commutative multiplication of *these* distributions such that resulting new Poisson brackets fulfil the standard requirements (antisymmetry and Jacobi identity).

The new Poisson brackets, of course, are reduced to the standard ones for those cases when all surface terms are zero. Really, the range of applicability of the standard brackets is even larger as it is clear from the successful Regge-Teitelboim approach [2]. They can be used if all supplementary terms appearing in the new brackets are zero due to boundary conditions (or, in other words, if Jacobi identity is still true). According to terminology of the book [1] the standard brackets are applicable only for "admissible functionals" whereas for the new ones all local functionals are admissible.

2 Notations and background

We use the local coordinate language and instead of a manifold with a boundary consider a domain Ω in R^n having a smooth boundary $\partial\Omega$. The characteristic function of this domain is $\theta_\Omega = \theta(P_\Omega)$, where equation $P_\Omega(x^1, ..., x^n) = 0$ defines the boundary.

Definition 2.1

An integral over a compact domain Ω of a function of field variables $\phi^A(x), A = 1, ..., p$ and their partial derivatives $D_J\phi^A$ up to some finite order

$$F = \int_\Omega d^n x f(\phi_A(x), D_J\phi_A(x))$$

is called a local functional.

All the functions f and ϕ_A as well as their variations are supposed infinitely smooth, i.e. $C^\infty(R^n)$. We use the multi-index notations $J = (j_1, ..., j_n)$

$$D_J = \frac{\partial^{|J|}}{\partial^{j_1}x^1 ... \partial^{j_n}x^n}, \qquad |J| = j_1 + ... + j_n.$$

Binomial coefficients for multi-indices are

$$\binom{J}{K} = \binom{j_1}{k_1} ... \binom{j_n}{k_n}.$$

As the number of sums in some formulae is large enough, we write only one sign of summing without displaying the indices of summation. Sum over all repeated indices should be understood. Only in those cases, where it is not so, we display the summation indices. Also, we do not show the limits of summation, because they are always natural, i.e. outside them the summand is simply zero. Such a nice property of binomial coefficients is exploited in many cases of changing of the orders of summation. There is also a temptation to remove $d^n x$ in the integrals and to write the arguments only if they can be mixed. let us use in parallel the notations

$$\int_\Omega f \qquad \text{or} \qquad \int \theta_\Omega f \qquad \text{or} \qquad \int \theta(P_\Omega) f.$$

We denote as $\mathcal{A}$ the space of local functionals . It is important that this space includes functionals with integrands depending on derivatives of arbitrary order [6]. Otherwise the Poisson brackets could go out of $\mathcal{A}$.

Definition 2.2
A bilinear operation $\{\cdot,\cdot\}$ *such that for any* $F, G, H \in \mathcal{A}$
1) $\{F, G\} \in \mathcal{A}$;
2) $\{F, G\} = -\{G, F\}$;
3) $\{\{F, G\}, H\} + \{\{H, F\}, G\} + \{\{G, H\}, F\} = 0$;
is called the new field theory Poisson bracket.

The standard Poisson bracket definition differs only by its irrelevance to divergencies.

Higher Eulerian operators E_A^J are defined [5] through the formula of the full variation of a local functional

$$\delta F = \sum \int_\Omega D_J\Big(E_A^J(f)\delta\phi_A\Big). \tag{2.1}$$

They can be given by the formula [5]

$$E_A^J(f) = \sum_K (-1)^{|K|+|J|}\binom{K}{J} D_{K-J}\frac{\partial f}{\partial \phi_A^{(K)}}. \tag{2.2}$$

Usual variational derivative (or Euler-Lagrange derivative) is the Eulerian operator of zeroth order. Let us mention that if J is not included into K, then all quantities having multi-index $(K-J)$ are zero. The sums over J in Eq.(2.1) and over K in Eq.(2.2) are really finite because a local functional can depend only on a finite number of derivatives.

3 Formulation of results

$$\{F, H\} = \sum \int_\Omega D_{J+K}\Big(E_A^J(f) I_{AB} E_B^K(h)\Big). \tag{3.1}$$

Theorem 3.1
Formula (3.1) *gives a new Poisson bracket if its zeroth order* ($|J| = 0 = |K|$) *term is a standard ultralocal Poisson bracket and the structure coefficients do not depend on the derivatives of the field variables.*

Remark. It is possible to include the case, when I_{AB} also depend on the field derivatives, but it makes the conditions for standard brackets not so transparent.

Let us remind that the standard field theory Poisson bracket [1]

$$\{F, G\} = \sum \int_\Omega \int_\Omega E_A^0(f(x)) E_B^0(g(y)) \{\phi_A(x), \phi_B(y)\}$$

can be derived, under assumption that all surface terms arising when integrating by parts are zero, from the formula

$$\{F, G\} = \sum \int_\Omega \int_\Omega \frac{\partial f}{\partial \phi_A^{(J)}(x)} \frac{\partial g}{\partial \phi_B^{(K)}(y)} \{D_J^{(x)}\phi_A(x), D_K^{(y)}\phi_B(y)\}, \tag{3.2}$$

or

$$\{F,G\} = \sum \int_\Omega \int_\Omega D_{f_A(x)} D_{g_B(y)} \{\phi_A(x), \phi_B(y)\},$$

where Fréchet derivatives

$$D_{f_A} = \sum_I \frac{\partial f}{\partial \phi_A^{(I)}} D_I. \tag{3.3}$$

are used.

Definition 3.2
The standard field theory Poisson bracket is called local if

$$\{\phi_A(x), \phi_B(y)\} = \frac{1}{2} \sum_L \Big(I^L_{AB}(x) D_L^{(x)} - I^L_{BA}(y) D_L^{(y)} \Big) \delta(x,y), \tag{3.4}$$

where the sum is of finite range in $|L|$.

Usually, derivatives over only one of the two arguments are present in the formulae like (3.4), because of the widely used relations

$$\Big(D_J^{(x)} - (-1)^{|J|} D_J^{(y)} \Big) \delta(x,y) = 0, \tag{3.5}$$

also accompanied by the conditions

$$I^L_{AB} = (-1)^{|L|+1} I^L_{BA}.$$

But if not all surface terms, arising in integration by parts, are zero, then Eq.(3.5) is not true. It is evident that the problem can be reduced to the problem of definition of the integrals like

$$\int_\Omega \int_\Omega f(x) g(y) D_J^{(x)} D_K^{(y)} \delta(x,y), \tag{3.6}$$

for finite domain when the test functions are nonzero on its boundary. So, here we propose a Rule which is in accordance with formula (3.1).

Rule 3.3

$$\int_\Omega \int_\Omega f(x) g(y) D_J^{(x)} D_K^{(y)} \delta(x,y) = \int_\Omega D_K f D_J g. \tag{3.7}$$

Taken together, Eqs.(3.2) and (3.7) give us a possibility to deduce not only the previously given expression (3.1) for ultralocal brackets, but also a more general result

$$\{F,G\} = \frac{1}{2} \sum \int_\Omega D_{P+Q} \Big(E^P_A(f) I^L_{AB} D_L E^Q_B(g) - (f \leftrightarrow g) \Big). \tag{3.8}$$

Theorem 3.4

The new Poisson brackets, corresponding to the standard local Poisson brackets with constant structure matrix, are given by formula (3.8).

Remark. The derivation does not restrict us to the case $I^L_{AB} = const$. But the proof of Jacobi identity becomes more difficult in the general case.

Let us present the standard variational, or Euler-Lagrange, derivative in the form

$$\frac{\delta F}{\delta \phi_A(x)} = E^0_A(f)\theta_\Omega.$$

Then it gives us a full variation

$$\delta F = \sum \int \frac{\delta F}{\delta \phi_A} \delta \phi_A,$$

of a local functional

$$F = \int \theta_\Omega f(\phi_A, D_J \phi_A),$$

only if all surface integrals in the general formula

$$\delta F = \sum \int \theta_\Omega D_J \Big(E^J_A(f) \delta \phi_A \Big),$$

are zero.

Definition 3.5

A distribution $\delta F / \delta \phi_A$ such that in general case, i.e. for arbitrary smooth variations $\delta \phi_A(x)$,

$$\delta F = \sum \int \frac{\delta F}{\delta \phi_A} \delta \phi_A, \tag{3.9}$$

will be called the full variational derivative of a local functional F.

Statement 3.6

The full variational derivative can be written in the form

$$\frac{\delta F}{\delta \phi_A} = \sum (-1)^{|J|} E^J_A(f) D_J \theta_\Omega, \tag{3.10}$$

where θ_Ω is a characteristic function of the domain of integration Ω.

Statement 3.7

By using Definition 3.5 *the expression* (3.8) *can be written in the form*

$$\{F, G\} = \sum \int \int \frac{\delta F}{\delta \phi_A(x)} \{\phi_A(x), \phi_B(y)\} \frac{\delta G}{\delta \phi_B(y)}, \tag{3.11}$$

if we admit the following multiplication rule:

Rule 3.8

$$D_J \theta(P_\Omega) \times D_K \theta(P_\Omega) = D_{J+K} \theta(P_\Omega).$$

Remark. Of course, this Rule has its domain of applicability only inside our procedure of calculating the Poisson brackets.

Statement 3.9
Rule 3.3 *is a corollary of* Rule 3.8.

Transcending the two cases covered by Theorems 3.1 and 3.4 for those we are able to prove Jacobi identity we intend to make in their extension a Hypothesis.

Hypothesis 3.10
The expression (3.8) *gives a new Poisson bracket for any local standard Poisson bracket* (3.4).

The new Poisson brackets can be written in different equivalent forms:

1) through the full (*not standard*) variational derivatives defined by the formula (3.10) and with account for Rule 3.8:

$$\{F,G\} = \sum \int\int \frac{\delta F}{\delta \phi_A(x)} \{\phi_A(x), \phi_B(y)\} \frac{\delta G}{\delta \phi_B(y)},$$

2) through higher Eulerian operators (2.2):

$$\{F,G\} = \frac{1}{2} \sum \int_\Omega D_{P+Q} \Big(E_A^P(f) \hat{I}_{AB} E_B^Q(g) - E_A^P(g) \hat{I}_{AB} E_B^Q(f) \Big),$$

where

$$\hat{I}_{AB} = \sum_N I_{AB}^N D_N,$$

3) through Fréchet derivatives (3.3):

$$\{F,G\} = \frac{1}{2} \sum \int_\Omega Tr(D_{f_A} \hat{I}_{AB} D_{g_B} - D_{g_A} \hat{I}_{AB} D_{f_B}),$$

4) through some matrix notations :

$$\{F,G\} = \frac{1}{2} \sum \int_\Omega \Big(\langle \nabla f \cdot C \nabla g \rangle - \langle \nabla g \cdot C \nabla f \rangle \Big),$$

defined below

$$(\nabla f)_{J,L,A} = D_L \frac{\partial f}{\partial \phi_A^{(J)}}, \qquad (\nabla g)_{K,M,B} = D_M \frac{\partial g}{\partial \phi_B^{(K)}},$$

$$C_{JK,LM,AB} = \binom{J}{L} \binom{K}{M} D_{J+K-L-M} \hat{I}_{AB}.$$

4 Proof of Jacobi identity

The detailed proofs of Jacobi identity for the new brackets are long enough in general cases of Theorems 3.1 and 3.4 and will be published in other place [7]. Here we demonstrate a proof for the simplest case of ultralocal bracket with constant coefficients.

Statement 4.1

For constant structure matrix the ultralocal Poisson bracket (3.1) *can be written in the form*

$$\{F, G\} = \sum \int_\Omega Tr(D_{f_A} I_{AB} D_{g_B}), \tag{4.1}$$

where D_{f_A} *is Fréchet derivative* (3.3), *and*

$$Tr(D_{f_A} I_{AB} D_{g_B}) = \sum I_{AB} D_J \frac{\partial f}{\partial \phi_A^{(I)}} D_I \frac{\partial g}{\partial \phi_B^{(J)}}.$$

Proof. Let us use the Leibnitz rule

$$D_J(fg) = \sum_K \binom{J}{K} D_K f D_{J-K} g \tag{4.2}$$

in Eq.(3.1)

$$\{F, G\} = \sum I_{AB} \binom{I+J}{M} \int_\Omega D_M E_A^I(f) D_{I+J-M} E_B^J(g).$$

By exploiting Eq.(2.2) it can be transformed to

$$\sum I_{AB} (-1)^{|I|+|K|+|J|+|L|} \binom{I+J}{M} \binom{K}{I} \binom{L}{J} \int_\Omega D_{M+K-I} \frac{\partial f}{\partial \phi_A^{(K)}} D_{I-M+L} \frac{\partial g}{\partial \phi_B^{(L)}}.$$

Then by changing the indices $M \to M + I$ and the order of summation with the help of combinatorial identities

$$\sum_{l=k}^{j} (-1)^l \binom{l}{i} \binom{j-k}{l-k} = (-1)^j \binom{k}{j-i}, \qquad \sum_{l=0}^{j} \binom{i}{l} \binom{j-k}{j-l} = \binom{i+j-k}{j},$$

we are able to estimate the sum

$$\sum_{I,J} (-1)^{|I|+|J|} \binom{I+J}{I+M} \binom{K}{I} \binom{L}{J} = (-1)^{|K|+|L|} \delta_{M,L-K}.$$

As a result we obtain Eq.(4.1).

Statement 4.2 *The Poisson bracket, given by formula* (3.1), *fulfils the Jacobi identity when* $I_{AB} = const$.

Proof. Let us transform the expression

$$\{\{F, G\}, H\} = \sum I_{AB} I_{CD} \int_\Omega D_I \frac{\partial h}{\partial \phi_B^{(J)}}$$

$$\times D_J\left(\frac{\partial}{\partial\phi_A^{(I)}}(D_K\frac{\partial f}{\partial\phi_C^{(L)}})D_L\frac{\partial g}{\partial\phi_D^{(K)}}+D_L\frac{\partial f}{\partial\phi_C^{(K)}}\frac{\partial}{\partial\phi_A^{(I)}}(D_K\frac{\partial g}{\partial\phi_D^{(L)}})\right),$$

with the help of relation [8]

$$\frac{\partial}{\partial\phi_A^{(I)}}D_J f=\sum_K\binom{J}{K}D_{J-K}\frac{\partial f}{\partial\phi_A^{(I-K)}},$$

Leibnitz rule (4.2) and antisymmetry over $C\leftrightarrow D$

$$\{\{F,G\},H\}=\sum\binom{K}{M}\binom{J}{N}I_{AB}I_{CD}$$

$$\times\int_\Omega\left(D_{K+N-M}\frac{\partial^2 f}{\partial\phi_A^{(I-M)}\partial\phi_C^{(L)}}D_I\frac{\partial h}{\partial\phi_B^{(J)}}D_{J+L-N}\frac{\partial g}{\partial\phi_D^{(K)}}\right.$$
$$\left.-D_{K+N-M}\frac{\partial^2 g}{\partial\phi_A^{(I-M)}\partial\phi_C^{(L)}}D_I\frac{\partial h}{\partial\phi_B^{(J)}}D_{J+L-N}\frac{\partial f}{\partial\phi_D^{(K)}}\right).$$

After cyclic permutation we have

$$\{\{F,G\},H\}+\{\{H,F\},G\}+\{\{G,H\},F\}$$
$$=\sum\binom{K}{M}\binom{J}{N}I_{AB}I_{CD}\int_\Omega D_{K+N-M}\frac{\partial^2 f}{\partial\phi_A^{(I-M)}\partial\phi_C^{(L)}}$$
$$\times\left(D_{J+L-N}\frac{\partial g}{\partial\phi_D^{(K)}}D_I\frac{\partial h}{\partial\phi_B^{(J)}}-(g\leftrightarrow h)\right)+\ldots,$$

where dots mean analogous terms with cyclically permuted f,g,h. By changing indices $N\to N+J$, $I\to I+M$, we get

$$\{\{F,G\},H\}+\{\{H,F\},G\}+\{\{G,H\},F\}=\sum\binom{K}{K-M}\binom{J}{J+N}I_{AB}I_{CD}$$

$$\times\int_\Omega D_{J+K+N-M}\frac{\partial^2 f}{\partial\phi_A^{(I)}\partial\phi_C^{(L)}}\left[D_{L-N}\frac{\partial g}{\partial\phi_D^{(K)}}D_{I+M}\frac{\partial h}{\partial\phi_B^{(J)}}-(g\leftrightarrow h)\right]+\ldots$$

So, if we simultaneously change $I\leftrightarrow L$, $J\leftrightarrow K$, $M\leftrightarrow -N$, $A\leftrightarrow C$ and $B\leftrightarrow D$, then the expression in square brackets changes its sign while the coefficient before the brackets stands as itself. Therefore, the sum equals zero, and the Jacobi identity is fulfilled in this simplest case.

5 Conclusion

It is clear that the above results can be applied to the field theory on manifolds with a boundary simply by postulating Rule 3.3 and independently of any reasoning about characteristic functions. The new Poisson structure permits to consider dynamical problems in which boundary values of the field variables are treated on equal footing with their internal values. The dynamics on the boundary is determined by both volume and surface parts of the Hamiltonian. Any choice of boundary conditions is in fact a constraint in the phase space and should be treated along with the standard procedure of searching for secondary and higher constraints. These boundary conditions do not interfere with the dynamical equations inside the domain until we start solving elliptic type constraints such as the Gauss law in gauge theories. Then the nonlocal dependence appears, including the dependence of surface variables, and the boundary part of the Hamiltonian begins to influence the equations of motion of internal variables.

In relation to the new brackets we now can see more questions than answers. The Jacobi identity for the most general case of local brackets is still not proved. It is not clear whether it is possible to generalize this construction onto nonlocal case. The global formulation is not elaborated. It is important to understand what class of functions should be exploited in searching for solutions of the Hamiltonian equations.

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