Total Divergences in Hamiltonian Formalism of Field Theory

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The field theory Hamiltonian formalism have been paid a lot of attention in the two previous decades due to studying of integrable models. Now the concepts of Poisson bracket and Hamiltonian operator are deeply elaborated, see for example Refs. 1,2.

But from physicist's viewpoint the treatment based on free integration by parts sometimes seems too restrictive. There are problems where surface integrals are nonzero and have physical meaning. We can mention characteristics of the gravitational field in asymptotically flat space-times,[3] surface energy of a fluid,[4] etc. As a result, in the cited works the concept of Poisson bracket is exploited outside of the definition given in Refs. 1,2 and in many other recent mathematical textbooks.

In this report it is proposed to generalize the definition of Poisson brackets in order to treat integrals of divergences as normal Hamiltonians which generate a kind of Hamiltonian equations on the boundary. Nonlinear Schrödinger equation is used as an illustrative example.

We use the local coordinate language and 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 1

An integral over a finite 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

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

is called a local functional.

All the functions f and ϕ_A as well as their variations are supposed to be 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

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

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. Otherwise the Poisson bracket could go out of $\mathcal{A}$.

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Definition 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[1,2] definitions of local functional and Poisson bracket differ only in adding words "modulo divergences".

It occurs possible to construct new expressions for field theory Poisson brackets fulfilling the new definition, by supposing locality and antisymmetry, i.e.

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

and these expressions are the same for all kinds of boundary conditions:

$$\frac{1}{2} \sum_{A,B,P,Q} \int\limits_\Omega D_{P+Q} \Big(E^P_A(f) \hat{I}_{AB} E^Q_B(g) - E^P_A(g) \hat{I}_{AB} E^Q_B(f) \Big) d^n x, \tag{1}$$

where

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

and coefficients I^N_{AB} satisfy some standard conditions[5]. Higher Eulerian operators E^J_A are defined in Ref. 1 through the formula of the full variation of a local functional

$$\delta F = \sum_{A,J} \int\limits_\Omega D_J \Big(E^J_A(f) \delta\phi_A \Big) d^n x.$$

They can be explicitly expressed as

$$E^J_A(f) = \sum_K (-1)^{|K|+|J|} \binom{K}{J} D_{K-J} \frac{\partial f}{\partial \phi^{(K)}_A}.$$

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 and K are really finite because a local functional can depend only on a finite number of derivatives.

The replacement of the old brackets by the new ones can be understood as a transition from functional variations with fixed values of the field on the boundary to free variations. Then a natural construction that we call a full variational derivative appears in the place of the standard Euler-Lagrange variational derivative. This new object cares information not only on the integrand (up to constants), but also on the domain of integration Ω

$$\frac{\delta F}{\delta \phi_A} = E^0_A(\theta_\Omega f) = \sum_J (-1)^{|J|} E^J_A(f) D_J \theta_\Omega,$$

where θ_Ω is a characteristic function of the domain.

Inserting this variational derivative into the standard formula

$$\{F, G\} = \sum_{A,B} \int\int \frac{\delta F}{\delta \phi_A(x)} \{\phi_A(x), \phi_B(y)\} \frac{\delta G}{\delta \phi_B(y)} d^n x d^n y,$$

we should formally integrate by parts separately in x and y variables to remove derivatives from the δ-function. Afterwards we take off one of the integrations naively with the help of δ-function and obtain an integral containing product of distributions. By mystical way it occurs that by using a formal rule

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

to transform integrand into the legal form and then integrating by parts over infinite region we get a formula (1) that satisfies the new definition of Poisson brackets given above.

Evidently to prove this statement we should prove Jacobi identity and for wide classes of local brackets this is done in Ref. 5.

Let us now consider a simple example of the Hamiltonian system and obtain boundary equations with the help of the new brackets. The nonlinear Schrödinger equation can be treated[6] as generated by the Hamiltonian

$$H = \frac{1}{2}\int(\mathcal{H} + \bar{\mathcal{H}})dx, \tag{2}$$

where

$$\mathcal{H} = r'q' + kr^2q^2, \qquad \bar{\mathcal{H}} = \bar{r}'\bar{q}' + k\bar{r}^2\bar{q}^2,$$

and Poisson brackets

$$\{q(x), r(y)\} = -2i\delta(x,y), \qquad \{\bar{q}(x), \bar{r}(y)\} = 2i\delta(x,y).$$

To return to the standard notations we should put reality conditions

$$\psi = q = \bar{r}, \qquad \bar{\psi} = r = \bar{q}.$$

By considering Poisson brackets for integrals of the full space derivatives of canonical variables $\phi_A = (q, r)$ with the Hamiltonian we expect to obtain dynamical equations on the boundary in functional form

$$\frac{d}{dt}\int {\phi_A}'dx = \{\int {\phi_A}'dx, H\} = \int D(\frac{1}{2}\sum_B I_{AB}\frac{\partial\mathcal{H}}{\partial\phi_B})dx.$$

If we try to use Newton-Leibnitz formula then we get

$$\dot{\phi_A}\Big|_1^2 = \frac{1}{2}\sum_B I_{AB}\frac{\partial\mathcal{H}}{\partial\phi_B}\Big|_1^2.$$

This is different from the standard (internal) equations

$$\dot{\phi_A} = \frac{1}{2}\sum_B I_{AB}E_B^0(\mathcal{H}).$$

For the given Hamiltonian the formal equations for boundary values are

$$\dot{q}_b = -2ikr_b{q_b}^2, \qquad \dot{r}_b = 2ik{r_b}^2q_b.$$

These equations can be easily integrated and give elementary oscillations at the ends:

$$\psi_b(t) = \psi_b(0)exp(-2ik|\psi_b(0)|^2t).$$

We can see that in this case the dynamics of boundary values is separated from the internal dynamics. Of course, this situation is not general.

But we should not understand this result too naively. Strictly speaking only Hamiltonian equations for functionals can be obtained. When another boundary functional

$$\int (f(\phi_A))' dx$$

is taken its bracket with the Hamiltonian is not equal to

$$(f(\phi_A))' \dot{\phi}_A(2) - (f(\phi_A))' \dot{\phi}_A(1).$$

Let us now demonstrate that usual canonical transformations involving space derivatives are not strictly canonical when divergence terms are taken into account. In Ref.6 a transformation

$$Q = \frac{1}{kr}, \qquad R = kr^2 q - r'' + \frac{r'^2}{r},$$

is exploited, which has an inverse

$$r = \frac{1}{kQ}, \qquad q = kQ^2 R - Q'' + \frac{Q'^2}{Q}.$$

By taking $\phi_A = (Q, R)$ let us estimate

$$\{\phi_A(x), \phi_B(y)\} = \frac{1}{2}(\hat{I}_{AB}(x) - \hat{I}_{BA}(y))\delta(x, y),$$

and find that

$$\hat{I}_{AB} = 2i \begin{pmatrix} 0 & -1 \\ 1 & -2D1/(kQ^2)D \end{pmatrix}$$

Therefore noncanonicity of the transformation appears in the bracket

$$\{R(x), R(y)\} = \frac{-2i}{k}(D_x \frac{1}{Q^2(x)} D_x - D_y \frac{1}{Q^2(y)} D_y)\delta(x, y).$$

The Hamiltonian in the new variables will be given by Eq.(2) where

$$\mathcal{H} = kQ^2 R^2 - Q'R' - 2Q''R + + \frac{1}{k}\Big[2\Big(\frac{Q'}{Q}\Big)^4 + \Big(\frac{Q''}{Q}\Big)^2 - 4\Big(\frac{Q'^2 Q''}{Q^3}\Big) + \frac{Q'Q'''}{Q^2}\Big].$$

We need to consider Hamiltonian equations for functionals

$$\begin{aligned} F_1 &= \int q' dx = \int \Big(kQ^2 R - Q'' + \frac{Q'^2}{Q}\Big)' dx, \\ F_2 &= \int r' dx = \int \Big(\frac{1}{kQ}\Big)' dx, \end{aligned}$$

which can be obtained by calculating the Poisson brackets

$$\{F, H\} = \{F, H\}_c + \{F, H\}_{nc},$$

where

$$\{F, H\}_c = -2i \sum_{m,n} \int D_{m+n} \Big(E_Q^m(F) E_R^n(H) - E_R^m(F) E_Q^n(H)\Big) dx, \tag{3}$$

$$\{F, H\}_{nc} = -\frac{2i}{k} \sum_{m,n} \int D_{m+n} \Big(E_R^m(F) D \frac{1}{Q^2} D E_R^n(H) - E_R^m(H) D \frac{1}{Q^2} D E_R^n(F)\Big) dx. \tag{4}$$

Evidently, noncanonical term appears only in calculation of $\{F_1, H\}$.

We first display here the higher Eulerian derivatives of H and F_1:

$$\begin{array}{llll}
E^0_R(H) = & kQ^2R - Q''/2, & E^0_R(F_1) = & 0, \\
E^1_R(H) = & -Q'/2, & E^1_R(F_1) = & kQ^2, \\
E^0_Q(H) = & -R''/2 + kQR^2, & E^0_Q(F_1) = & 0, \\
E^1_Q(H) = & 3/2R' + Q'^3/(kQ^4) - Q'Q''/(kQ^3), & E^1_Q(F_1) = & 2kQR + (Q'/Q)^2 - 2Q''/Q, \\
E^2_Q(H) = & -R + Q'^2/(kQ^3) - Q''/(2kQ^2), & E^2_Q(F_1) = & 2Q'/Q, \\
E^3_Q(H) = & Q'/(2kQ^2), & E^3_Q(F_1) = & -1.
\end{array}$$

Then we present the result of calculation for noncanonical term (4):

$$-2i \int D\Big(-Q'''' + 3Q'''Q'/Q + 3Q''^2/Q - 6Q''Q'^2/Q^2 + 2Q'^4/Q^3 + 2kQQ'R' + kQ^2R''\Big)dx.$$

Only taking this term into account we are getting for $\{F_1, H\}$ a result which is equivalent to the one obtained in old variables.

In one of our previous publications[7] we already have discussed this problem in relation to Ashtekar's canonical transformation in General Relativity. But there the standard definition of Poisson bracket was used and so Jacobi identity was not granted to be fulfilled in general case. To get the correct result one must repeat that calculation in the new brackets.

References

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