About Boundary Terms in Higher Order Theories

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Abstract: It is shown that when in a higher order variational principle one fixes fields at the boundary leaving the field derivatives unconstrained, then the variational principle (in particular the solution space) is not invariant with respect to the addition of boundary terms to the action, as it happens instead when the correct procedure is applied. Examples are considered to show how leaving derivatives of fields unconstrained affects the physical interpretation of the model. This is justified in particularl by the need of clarifying the issue for the purpose of applications to relativistic gravitational theories, where a bit of confusion still exists. On the contrary, as it is well known for variational principles of order k, if one fixes variables together with their derivatives (up to order $k-1$) on the boundary then boundary terms leave solution space invariant.

1. Introduction

Recently the interest in higher order Lagrangian theories has been renewed within the framework of covariant field theories in various contexts, aiming to suitably extend standard (Hilbert-Einstein) General Relativity in order to model, at least partially, dark energy/matter effects (see **[1]** and references quoted therein) via the use of gravitational Lagrangians depending non-linearly on the curvature.

In gravitational literature different attitudes towards boundary conditions in GR and in alternative gravitational theories are presented (see **[2]** for a detailed review). We shall here stress that mathematical consequences of different attitudes must be considered *before* any physical interpretation is attempted and that of course one is not free to ignore these consequences, that might be (and usually are) rather crucial for a number of physically relevant issues, e.g. the definition of conservation laws and their correct physical interpretation.

From the mathematical viewpoint, any attitude towards boundary conditions should be dictated by Hamilton's least action principle. This principle is a *definition* of the critical sections which have to be understood as physical configurations. Being it a *definition* one is logically free to choose the formulation which is more suitable to the situation. However, there are physical and mathematical consequences of this choice which must be in any case taken into account. Moreover, it would be appreciated if a general guiding principle would avoid to treat each model on its own on the base of physical considerations which in some cases (e.g. when dealing with exotic physics or non-trivial generalizations of the models already considered) could be unclear.

In particular, we shall hereafter show that if one assumes that only the value of fields must be fixed while (higher order) derivatives are left unconstrained at the boundary, then one cannot keep that pure divergencies in the action leave the solution space invariant, as it happens in the standard applications of Calculus of Variations. This is particularly relevant for Gravity, since in the literature (see e.g. **[3]**) it is often claimed that in standard GR one is free to choose not to fix first derivatives of the metric at the boundary, since the boundary terms of the Hilbert

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action can be written as a total variation and hence can be compensated in various non-unique ways by adding suitable boundary terms to the action. Even if this is mathematically correct in GR it is in any case rather misleading since such a procedure fails to hold if one considers Lagrangians that are non-degenerate and non-linear in curvature. Accordingly we believe that whenever such a choice is adopted one should clearly state that this is done at the expense of *changing* the space of solutions and affecting conservation laws which is unfortunately physically disturbing; see also [**4**].

As a motivation for such an uncanonical choice it is often claimed that fixing higher order variations of the fields may affect their physical interpretation so that this standard attitude should not be embraced without considering these effects. This is of course true and we fully agree that detailed discussions on the role that different boundary conditions have in GR is extremely important. However, it is also true the other way around, i.e. when leaving variations of field derivatives free at the boundary one should always be careful about the change of solution space, the interpretation of boundary fluxes as well as the further spurious boundary equations that appear besides the (bulk) field equations.

Hereafter, we shall present explicit examples in Mechanics and Field Theory. From these examples it is clearly shown that if one artificially wants to describe a system by a higher order Lagrangian adding pure divergencies to the Lagrangian itself, then in order to maintain the standard interpretation of the physical system one is forced to fix variations *and their derivatives* at the boundary. The examples will in fact show, *en passant*, how the solution space may drastically change and even reduce to empty if the standard procedures of Calculus of Variations are not used.

2. The Relation between Higher Order Variations and Boundary Terms

Let us consider the following Lagrangian

$$L'(q,\dot q,\ddot q) = \dot q\ddot q + \frac{1}{2}\left(\dot q^2 - \omega^2\, q^2\right) + \omega^2 q\dot q \tag{2.1}$$

which is easily found to be equivalent to the Lagrangian of an harmonic oscillator and to give rise to the same dynamics via Euler-Lagrange equations (of order 2). Varying it we have

$$\begin{aligned}\delta L' &= \delta\dot q\ddot q + \dot q\delta\ddot q + \dot q\,\delta\dot q - \omega^2\, q\,\delta q + \omega^2\delta q\dot q + \omega^2 q\delta\dot q = \\ &= \tfrac{d}{dt}\left(\delta q\ddot q\right) - \delta q\tfrac{d^3q}{dt^3} + \tfrac{d}{dt}\left(\dot q\delta\dot q\right) - \tfrac{d}{dt}\left(\ddot q\delta q\right) + \tfrac{d^3q}{dt^3}\delta q + \\ &\quad + \tfrac{d}{dt}\left(\dot q\,\delta q\right) - \ddot q\,\delta q - \omega^2\, q\,\delta q + \omega^2\delta q\dot q + \tfrac{d}{dt}\left(\omega^2 q\delta q\right) - \omega^2\dot q\delta q = \\ &= \tfrac{d}{dt}\left(\dot q\delta\dot q + \left(\dot q + \omega^2 q\right)\delta q\right) - \left(\ddot q + \omega^2\, q\right)\ \delta q\end{aligned} \tag{2.2}$$

If following the standard prescriptions of Calculus of Variations we assume $\delta q = 0$ and $\delta\dot q = 0$ on the boundary of an interval $[t_0, t_1]$ then we obtain in fact the equation of motion of the $1d$-harmonic oscillator

$$\ddot q + \omega^2\, q = 0 \tag{2.3}$$

This is no mistery since the Lagrangian (2.1) can be easily recasted as follows

$$L'(q,\dot q,\ddot q) = \frac{1}{2}\left(\dot q^2 - \omega^2\, q^2\right) + \frac{d}{dt}\left(\frac{1}{2}\ \left(\dot q^2 + \omega^2 q^2\right)\right) \tag{2.4}$$

so that it manifestly differs from the harmonic oscillator Lagrangian $L(q,\dot q) = \frac{1}{2}\left(\dot q^2 - \omega^2\, q^2\right)$ by a total time derivative (which is the mechanical equivalent of a pure divergence term in field theory). Hence, in this case, we know that the pure-divergence-term $\frac{d}{dt}\left(\frac{1}{2}\,\left(\dot q^2 + \omega^2 q^2\right)\right)$ in the Lagrangian L' is totally unessential with respect to the equation of motion. Let us stress that in this case the pure divengence term is even zero on-shell because of the conservation of total energy, since the boundary term is nothing but the total derivative of the Hamiltonian.

If one decides instead to fix only $\delta q = 0$ on the boundary, leaving $\delta\dot q$ unfixed, then extra boundary field equations are added in order to kill the extra boundary contribution to the action. The equations of motion that follow form (2.2) in this case are

$$\begin{cases} \ddot q + \omega^2\, q = 0 \\ \dot q_0 = 0 \end{cases} \tag{2.5}$$

which in fact admit less solutions than Eq. (2.3). Notice that solutions to this problem are in fact just a zero-measure set in the solution space of the $1d$-harmonic oscillator!

If one decides not to keep the first derivatives fixed, by adding pure divergencies one can even invent nastier and nastier examples. For instance, by considering the following 1-parameter family of Lagrangians

$$L''(q,\dot q,\ddot q;\Lambda) = \frac{1}{2}\left(\dot q^2 - \omega^2\, q^2\right) + \frac{d}{dt}\left(\frac{1}{6}\,\dot q^3 + \left(\frac{\omega^2}{2}\, q^2 + \Lambda^2\right)\dot q\right) \tag{2.6}$$

with Λ real, which produce equations of motion in the form

$$\begin{cases} \ddot q + \omega^2\, q = 0 \\ \dot q_0^2 + \omega^2 q_0^2 = -\Lambda^2 \end{cases} \tag{2.7}$$

wee see that, for any $\Lambda \neq 0$, one has no solution at all, since there are no initial conditions satisfying the boundary equation. And even for $\Lambda = 0$ the solution space is much smaller than the solution space of the harmonic oscillator, since it reduces again to quiet.

3. Examples in GR

Of course one could argue that field theory is not Mechanics and that in Field Theory there is more space to play with. Such an assumption is of course true, but still one has to pay a lot of attention when playing. . . ! Let us then present similar situations in GR.

Let M be a 4-dimensional manifold with boundary Ω and let us consider the metric Lagrangian

$$L = \sqrt{g}R - \nabla_\alpha\left(\sqrt{g}g^{\mu\nu}\left(u^\alpha_{\mu\nu} - \bar u^\alpha_{\mu\nu}\right)\right) = \left[\sqrt{g}g^{\alpha\beta}(\Gamma^\rho_{\alpha\sigma}\Gamma^\sigma_{\rho\beta} - \Gamma^\sigma_{\sigma\rho}\Gamma^\rho_{\alpha\beta}) + d_\sigma(\sqrt{g}g^{\alpha\beta}\bar u^\sigma_{\alpha\beta})\right] ds \tag{3.1}$$

where: ds is the standard local volume element induced by the coordinates; here and below, $\Gamma^\alpha_{\beta\mu}$ are the coefficients of the Levi-Civita connection of the metric g; we set $u^\lambda_{\mu\nu} = \Gamma^\lambda_{\mu\nu} - \delta^\lambda_{(\mu}\Gamma^\alpha_{\nu)\alpha}$ and $\bar u^\lambda_{\mu\nu} = \bar\Gamma^\lambda_{\mu\nu} - \delta^\lambda_{(\mu}\bar\Gamma^\alpha_{\nu)\alpha}$ for any connection $\bar\Gamma^\lambda_{\mu\nu}$ chosen at will on M. $\Gamma^\alpha_{\beta\mu}$ as well as $u^\lambda_{\mu\nu}$ are functions of the first derivatives of the field $g_{\mu\nu}$, while $\bar\Gamma^\lambda_{\mu\nu}$ is just a "fixed parametrization" i. e. a non-dynamical background (as one could easily see by realizing that the Euler-Lagrange equations of (3.1) with respect to $\bar\Gamma^\lambda_{\mu\nu}$ are identities). As long as the background connection

$\bar{\Gamma}^{\alpha}_{\beta\mu}$ is considered, one is free to fix it at will: it can be a generic connection or the Levi-Civita connection of a background metric $\bar{g}$ (which could even have in principle a different signature) depending on the situation.

The Lagrangian (3.1) is covariant and first order in $g_{\mu\nu}$; the connection $\bar{\Gamma}^{\alpha}_{\beta\mu}$ is not subjected to any field equations so that it can be any connection both *a priori* and *a posteriori* (we stress that connections exist globally on any manifold); bulk field equations for g are vacuum Einstein field equations.

The background $\bar{u}^{\lambda}_{\mu\nu}$ is here added to preserve covariance. One could fix coordinates so that $\bar{u}^{\lambda}_{\mu\nu} = 0$ (usually at a point), or consider a fixed $\bar{u}^{\lambda}_{\mu\nu}(x)$ as a point dependence (we stress that it is relegated into a divergence). Our procedure is analogous to the one used by Hawking and Ellis (see **[5]**) to study the Cauchy problem in Relativity; there a background (metric) is used at the level of field equations, to show essential hyperbolicity, while here it is used at the level of the action. The two approaches are equivalent since the background is non-dynamical and its fixing commutes with the derivation of field equations; see also **[6]**.

The variation of this Lagrangian is given by

$$\delta L = \sqrt{g} G_{\mu\nu} \delta g^{\mu\nu} - \nabla_{\lambda} \left(\sqrt{g} (\delta^{\mu}_{(\alpha} \delta^{\nu}_{\beta)} - \tfrac{1}{2} g_{\alpha\beta})(u^{\lambda}_{\mu\nu} - \bar{u}^{\lambda}_{\mu\nu}) \delta g^{\alpha\beta} - \sqrt{g} g^{\mu\nu} \delta \bar{u}^{\lambda}_{\mu\nu} \right) \tag{3.2}$$

with $G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} R g_{\mu\nu}$. Applying standard techniques of Calculus of Variation one obtains only the bulk standard field equations $G_{\mu\nu} = 0$. If, instead, one fixes only $\delta g^{\mu\nu} = 0$ on the boundary, then a new boundary equation (associated to $\delta \bar{u}^{\lambda}_{\mu\nu}$) is added

$$\sqrt{g} g^{\mu\nu}|_{\Omega} = 0 \qquad \Rightarrow g_{\mu\nu}|_{\Omega} = 0 \tag{3.3}$$

This boundary condition is not only incompatible with the bulk field equations, but with kinematics in the first place (metrics are assumed in fact to be non-degenerate so that they are everywhere forbidden to vanish). Hence if one considers the Lagrangian (3.1), that differs from standard GR by a divergence, and fixes the metric only, then the solution space is *empty*!

One could argue that the background $\bar{u}^{\lambda}_{\mu\nu}$ is unphysical since it has no dynamics and that therefore there is no need to consider its variations. That is certainly reasonable though the argument can be reversed: since the field $\bar{u}^{\lambda}_{\mu\nu}$ is unphysical, then physics should be independent of how one decides to treat it: keeping it fixed or varying it, possibly varying an underlying metric $\bar{g}_{\mu\nu}$ that fixes it on the boundary, alone or together with its first derivative. The above example shows instead how the physical predictions of the theory (in particular the solution space) do depend on which unphysical degree of freedom is kept fixed on the boundary. Moreover, conservation laws would result to be affected by terms ensuing form the divergence (they can be easily calculated as in **[6]**).

Similar (but nastier) examples can be considered: e.g. the Lagrangian

$$L' = \sqrt{g} R - \tfrac{1}{\Lambda} \nabla_{\alpha} \left(\sqrt{g} g^{\mu\nu} R \left(u^{\alpha}_{\mu\nu} - \bar{u}^{\alpha}_{\mu\nu} \right) \right) \tag{3.4}$$

that is again classically equivalent to the Hilbert Lagrangian. The variation is now

$$\begin{aligned} \delta L' =& \sqrt{g} G_{\mu\nu} \delta g^{\mu\nu} - \nabla_{\lambda} \left(\tfrac{1}{\Lambda} \delta(\sqrt{g} g^{\mu\nu}) R \left(u^{\lambda}_{\mu\nu} - \bar{u}^{\lambda}_{\mu\nu} \right) + \tfrac{1}{\Lambda} \delta R \sqrt{g} g^{\mu\nu} \left(u^{\lambda}_{\mu\nu} - \bar{u}^{\lambda}_{\mu\nu} \right) \right) + \\ & - \nabla_{\lambda} \left(\tfrac{1}{\Lambda} \sqrt{g} g^{\mu\nu} (R - \Lambda) \delta u^{\lambda}_{\mu\nu} - \tfrac{1}{\Lambda} \sqrt{g} g^{\mu\nu} R \delta \bar{u}^{\lambda}_{\mu\nu} \right) \end{aligned} \tag{3.5}$$

Here, if we fix $\delta g^{\mu\nu} = 0$ leaving δR, $\delta u^\lambda_{\mu\nu}$ and $\delta \bar{u}^\lambda_{\mu\nu}$ unconstrained on the boundary, we have three boundary field equations

$$\begin{cases} \sqrt{g} g^{\mu\nu} \left(u^\alpha_{\mu\nu} - \bar{u}^\alpha_{\mu\nu} \right) \delta R|_\Omega = 0 \quad \Rightarrow u^\alpha_{\mu\nu}|_\Omega = \bar{u}^\alpha_{\mu\nu}|_\Omega \\ \sqrt{g} g^{\mu\nu} (R - \Lambda) \delta u^\lambda_{\mu\nu}|_\Omega = 0 \quad \Rightarrow R|_\Omega = \Lambda \\ g^{\mu\nu} R \delta \bar{u}^\lambda_{\mu\nu}|_\Omega = 0 \quad \Rightarrow R|_\Omega = 0 \end{cases} \tag{3.6}$$

As in the previous example, these three conditions are incompatible and the resulting solution space is again empty. Unlike the previous example, however, if in this case one decides not to vary the background the first two equations in (3.6) are still obtained along with Einstein equation; they (in particular, the second one) are enough to force the solution space to be empty. Here the troubles are generated exactly from not fixing $\delta u^\lambda_{\mu\nu}$ at the boundary. If now one adds to the Lagrangian a divergence that suitably counterbalance the first constraint, then this is enough, for any $\Lambda \neq 0$, to prevent Minkowski spacetime from being a solution of the theory, with a devastating effect on Newtonian limit and the physical interpretation of the whole theory.) The first condition imposes in fact to $g_{\mu\nu}$ an arbitrary asymptotic; if $\bar{u}^\lambda_{\mu\nu}$ is suitably chosen, then one could impose to $g_{\mu\nu}$ to be asymptotically AdS, dS or anything else. In any case, the solution space is again *empty*!

Other even more complicated examples can be studied under the form

$$L_f = \sqrt{g} R - \nabla_\alpha \left(\sqrt{g} g^{\mu\nu} f(R; \Lambda, \dots) \left(u^\alpha_{\mu\nu} - \bar{u}^\alpha_{\mu\nu} \right) \right) \tag{3.7}$$

We stress that of course there are reasonable boundary terms which do not force the solution space to be empty, but there is no guiding principle helping one in distinguishing good boundary terms from bad ones, so that such a procedure should be better avoided (being misleading) or, if really necessary, treated with the correct mathematical instruments. All this in the case that the "real" Lagrangian we start deforming is the Hilbert Lagrangian, that is known to be the only non-trivial second order Lagrangian linear in the curvature of a metric field. Linearity implies Hamiltonian degeneracy, so that the second order theory is essentially equivalent to a first order theory with second order field equations. It is exactly this degeneracy and the existence of a family of covariant first order (see [**6**]) that allows one to play with a certain success with the addition of divergencies. One should be aware that such a method *cannot* hold any longer in more general families of gravitational theories, such as e. g. all $f(R)$, Gauss-Bonnet, Lovelock, Chern-Simons Lagrangians and so on, including all effective Lagrangians that ensue from low limits of spacetime and/or quantum requirements.

4. Conclusions

We have here considered two attitudes in a variational principle of order k. Let us summarize our point. A *weakly critical configuration* is a configuration that extremizes the action for any deformation which vanishes along the boundary (while the field derivatives are left unconstrained).

A *critical configuration* is instead a configuration which extremizes the action for any deformation which vanishes together with its derivatives (up to order $k-1$) along the boundary.

Of course a weakly critical configuration is also critical, while the converse is false in general. From these simple examples we may easily conclude that, in a theory of order k, pure-divergence-terms may be considered unessential with respect to the field equations *only if* one considers critical configurations. On the contrary, by adding boundary terms to the action one can easily force the space of weakly critical configurations to be smaller or even empty.

Of course one is free to abandon the invariance of the action with respect to boundary contributions (as in a sense is done in the Hamiltonian formalism). Unfortunately, such an attitude strongly impacts on conservation laws which are an essential part of the physical interpretation of the theory as well.

Weakly critical configurations are considered in **[3]** (against the standard results in Variational Calculus and other important monographs in GR that more correctly consider only critical configurations; see **[5]**, **[7]**, **[8]**). In our opinion there is no real reason to impose an often artificial boundary term to a covariant action, breaking general covariance, in order to allow more general deformations of fields. Deformations in Lagrangian formalism have indeed no physical meaning. In Mechanics they are called in fact *virtual* dispacements also to stress the fact that they are not physical and they just need to be generically independent.

Any procedure that fixes fileds and no derivatives at the boundary is certainly very similar (if not technically identical) to a gauge fixing. Gauge fixing are useful in practice in special situations but there is no reason to break gauge covariance by fixing a gauge when a gauge covariant procedure allows to obtain the same result from a more fundamentally satisfactory point of view.

Another way of considering these examples is from control theory in the Hamiltonian framework. Boundary terms of the action are exactly the way of mimiking control theory at the Lagrangian level. In such a framework one is not concerned with computing physical configurations (namely, solutions of field equations) but how (and whether) physical configurations can respond to some constraint imposed at the boundary. For example, computing the electric field in a space with a conductor, knowing that the boundary, i.e. the surface of the conductor, is equipotential.

In this context the extra boundary equations are exactly interpreted as the condition one wishes to impose at the boundary. Here (and only here) one should guarantee that the boundary conditions imposed can be physically realized. It is no surprise that in certain cases there exist no configuration obeying those boundary conditions, meaning that one cannot physically impose those particular boundary conditions.

We have to stress that in gravitational experiments we are now technologically unable to impose *any* boundary conditions. It is therefore interesting to know that some requirements are forbidden in principle.

We have also to stress that the framework of control theory is by no means related to the determination of solutions of field equations, where by definition one wants to obtain *all* possible field configurations. Moreover, if we *unnecessarily* rely on boundary terms to obtain field equations, then this freedom cannot be exploited to deal with conservation laws (see **[9]**). In fact, it is well–known that, although divergencies leave invariant critical configurations, they affect conservation laws and conserved quantities that are an important part of the physical interpretation of the model. If boundary terms are fixed for field equations one could only hope conservation laws to turn out to make sense.

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