Boundary conditions play a crucial role in the path-integral approach to quantum gravity and quantum cosmology, as well as in the current attempts to understand the one-loop semiclassical properties of quantum field theories. Within this framework, one is led to consider boundary conditions completely invariant under infinitesimal diffeomorphisms on metric perturbations. These are part of a general scheme, which can be developed for Maxwell theory, Yang–Mills Theory, Rarita–Schwinger fields and any other gauge theory. A general condition for strong ellipticity of the resulting field theory on manifolds with boundary is here proved, following recent work by the authors. The relevance for Euclidean quantum gravity is eventually discussed.

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Foundational problems in quantum gravity

In several branches of classical and quantum field theory, as well as in the current attempts to develop a quantum theory of the universe and of gravitational interactions, it remains very useful to describe physical phenomena in terms of differential equations for the variables of the theory, supplemented by boundary conditions for the solutions of such equations. For example, the problems of electrostatics, the analysis of waveguides, the theory of vibrating membranes, the Casimir effect, van der Waals forces, and the problem of how the universe could evolve from an initial state, all need a careful assignment of boundary conditions. In the latter case, if one follows a path-integral approach, one faces two formidable tasks.

(i) the classification of the geometries occurring in the “sum over histories” and matching the assigned boundary data;

(ii) the choice of boundary conditions on metric perturbations which may lead to the evaluation of the one-loop semiclassical approximation. Indeed, while the full path integral for quantum gravity is a fascinating idea but remains a formal tool, the one-loop calculation may be put on solid ground, and appears particularly interesting because it yields the first quantum corrections to the underlying classical theory (despite the well known lack of perturbative renormalizability of quantum gravity based on Einstein’s theory). Within this framework, it is of crucial importance to understand whether the property of strong ellipticity of the boundary-value problem (see Appendix) is compatible with the request of local and gauge-invariant boundary conditions for a self-adjoint operator on perturbations.

For this purpose, we are now going to study gauge-invariant boundary conditions in a general gauge theory, following Ref. [1]. Given a Riemannian manifold $M$, a gauge theory is defined by two vector bundles, $V$ and $G$, such that $\dim V > \dim G$. $V$ is the bundle of gauge fields $\varphi \in C^\infty(V, M)$, and $G$ is the bundle of parameters of gauge transformations $\epsilon \in C^\infty(G, M)$. Both bundles $V$ and $G$ are equipped with some Hermitian positive-definite metrics $E$, $E^\dagger = E$, and $\gamma$, $\gamma^\dagger = \gamma$, and with the corresponding natural $L^2$ scalar products $(,)_V$ and $(,)_G$.

The infinitesimal gauge transformations

$$\delta \varphi = R\epsilon$$

are generated by a first-order differential operator $R$,

$$R : C^\infty(G, M) \to C^\infty(V, M).$$
Furthermore, two auxiliary operators are introduced,

\[ X : C^\infty(V, M) \to C^\infty(G, M) \]  

and

\[ Y : C^\infty(G, M) \to C^\infty(G, M), \]  

which make it possible to define the differential operators

\[ L \equiv XR : C^\infty(G, M) \to C^\infty(G, M) \]  

and

\[ H \equiv \bar{X}YX : C^\infty(V, M) \to C^\infty(V, M), \]  

where \( \bar{X} \equiv E^{-1}X^{\dagger}\gamma \). The operators \( X \) and \( Y \) should satisfy the following conditions (but are otherwise arbitrary):

1. The differential operators \( L \) and \( H \) have the same order.
2. The operators \( L \) and \( H \) are formally self-adjoint (or anti-self-adjoint).
3. The operators \( L \) and \( Y \) are elliptic.

From these conditions, two essentially different cases are found:

**Case I.** \( X \) is of first order and \( Y \) is of zeroth order, i.e.

\[ X = \bar{R}, \quad Y = I_G, \]  

where \( \bar{R} \equiv \gamma^{-1}R^{\dagger}E \). Then, of course, \( L \) and \( H \) are both second-order differential operators,

\[ L = \bar{RR}, \quad H = R\bar{R}. \]  

**Case II.** \( X \) is of zeroth order and \( Y \) is of first order. Let \( R \) be the bundle of maps of \( G \) into \( V \), and let \( \beta \in \mathcal{R} \) be a zeroth-order differential operator. Then

\[ X = \bar{\beta}, \quad Y = \beta R, \]  

where \( \bar{\beta} \equiv \gamma^{-1}\beta^{\dagger}E \), and the operators \( L \) and \( H \) are of first order,

\[ L = \bar{\beta}R, \quad H = \beta\bar{\beta}R\bar{\beta} = \beta L\bar{\beta}. \]
We assume that, by suitable choice of the parameters, the second-order operator $\bar{R}R$ can be made of Laplace type and the first-order operator $\bar{\beta}R$ can be made of Dirac type, and, therefore, have non-degenerate leading symbols (here denoted by $\sigma_L$)

\begin{align}
\det_{G}\sigma_L(\bar{R}R) & \neq 0, \\
\det_{G}\sigma_L(\bar{\beta}R) & \neq 0.
\end{align}

The dynamics of gauge fields $\varphi \in C^\infty(V,M)$ at the linearized (one-loop) level is described by a formally self-adjoint (or anti-self-adjoint) differential operator,

$$
\Delta : C^\infty(V,M) \to C^\infty(V,M).
$$

This operator is of second order for bosonic fields and of first order for fermionic fields. In both cases its leading symbol satisfies the identities

$$
\Delta R = 0, \quad \bar{R}\Delta = 0,
$$

and, therefore, is degenerate.

We consider only the case when the gauge generators are \textit{linearly independent}. This means that the equation

$$
\sigma_L(R)\epsilon = 0,
$$

has the only solution $\epsilon = 0$. In other words,

$$
\operatorname{Ker} \sigma_L(R) = \emptyset,
$$

i.e. the rank of the leading symbol of the operator $R$ equals the dimension of the bundle $G$,

$$
\operatorname{rank} \sigma_L(R) = \dim G.
$$

We also assume that the leading symbols of the generators $R$ are \textit{complete} in that they generate all zero-modes of the leading symbol of the operator $\Delta$, i.e. all solutions of the equation

$$
\sigma_L(\Delta)\varphi = 0,
$$

have the form

$$
\varphi = \sigma_L(R)\epsilon,
$$

for some $\epsilon$. In other words,

$$
\operatorname{Ker} \sigma_L(\Delta) = \{\sigma_L(R)\epsilon \mid \epsilon \in G\}.
$$
and hence
\[ \text{rank } \sigma_L(\Delta) = \dim V - \dim G. \] (21)

Furthermore, let us take the operator $H$ of the same order as the operator $\Delta$ and construct a formally (anti-)self-adjoint operator,
\[ F \equiv \Delta + H, \] (22)
so that
\[ \sigma_L(F) = \sigma_L(\Delta) + \sigma_L(H). \] (23)

It is easy to derive the following result:

The leading symbol of the operator $F$ is non-degenerate, i.e.
\[ \det_V \sigma_L(F) \neq 0. \] (24)

**Proof.** Indeed, suppose there exists a zero-mode $\varphi_0$ of the leading symbol of the operator $F$, i.e.
\[ \sigma_L(F)\varphi_0 = \bar{\varphi}_0\sigma_L(F) = 0, \] (25)
where $\bar{\varphi} \equiv \varphi^\dagger E$. Then we have
\[ \bar{\varphi}_0\sigma_L(F)\sigma_L(R) = \bar{\varphi}_0\sigma_L(\bar{X}Y)\sigma_L(L) = 0, \] (26)
and, since $\sigma_L(L)$ is non-degenerate,
\[ \bar{\varphi}_0\sigma_L(\bar{X}Y) = \sigma_L(YX)\varphi_0 = 0. \] (27)

But this implies
\[ \sigma_L(H)\varphi_0 = 0, \] (28)
and hence
\[ \sigma_L(F)\varphi_0 = \sigma_L(\Delta)\varphi_0 = 0. \] (29)

Thus, $\varphi_0$ is a zero-mode of the leading symbol of the operator $\Delta$, and according to the completeness of the generators $R$ must have the form $\varphi_0 = \sigma_L(R)\epsilon$ for some $\epsilon$. Substituting this form into Eq. (27) we obtain
\[ \sigma_L(YX)\sigma_L(R)\epsilon = \sigma_L(YL)\epsilon = 0. \] (30)
Herefrom, by taking into account the non-singularity of $\sigma_L(YL)$, it follows $\epsilon = \varphi_0 = 0$, and hence the leading symbol of the operator $F$ has no zero-modes, i.e. it is non-degenerate.

Thus, the operators $L$ and $F$ have, both, non-degenerate leading symbols. In quantum field theory the operator $X$ is called the gauge-fixing operator, $F$ the gauge-field operator, the operator $L$ the (Faddeev–Popov) ghost operator and the operator $Y$ in the Case II the third (or Nielsen–Kallosh) ghost operator. The most convenient and the most important case is when, by suitable choice of the parameters it turns out to be possible to make both the operators $F$ and $L$ either of Laplace type or of Dirac type. The one-loop effective action for gauge fields is given by the functional superdeterminants of the gauge-field operator $F$ and the ghost operators $L$ and $Y$:

$$\Gamma = \frac{1}{2} \log(\det F) - \log(\det L) - \frac{1}{2} \log(\det Y).$$ (31)

Let us now focus on bosonic fields, when $\Delta$ is a second-order formally self-adjoint operator. The gauge invariance identity (14) means, in particular,

$$\sigma_L(\Delta)\sigma_L(R) = 0.$$ (32)

Now we assume that both the operators $L = R R$ and $F = \Delta + R R$ are of Laplace type, i.e.

$$\sigma_L(R R) = |\xi|^2 I_G,$$ (33)

$$\sigma_L(F) = \sigma_L(\Delta) + \sigma_L(R R) = |\xi|^2 I_V.$$ (34)

On manifolds with boundary one has to impose some boundary conditions to make these operators self-adjoint and elliptic. They read

$$B_L \psi(\epsilon) = 0,$$ (35)

$$B_F \psi(\varphi) = 0,$$ (36)

where $\psi(\epsilon)$ and $\psi(\varphi)$ are the boundary data (see Appendix) for the bundles $G$ and $V$, respectively, and $B_L$ and $B_F$ are the corresponding boundary operators. In gauge theories one tries to choose the boundary operators $B_L$ and $B_F$ in a gauge-invariant way, so that the condition

$$B_F \psi(Re) = 0$$ (37)

is satisfied identically for any $\epsilon$ subject to the boundary conditions (35). This means that the boundary operators $B_L$ and $B_F$ satisfy the identity

$$B_F [\psi, R] (I_G - B_L) \equiv 0,$$ (38)
where \([\psi, R] \equiv \psi R - R\psi\).

We will see that this requirement fixes completely the form of the as yet unknown boundary operator \(B_L\). Indeed, the most natural way to satisfy the condition of gauge invariance is as follows. Let us decompose the cotangent bundle \(T^*(M)\) in such a way that \(\xi = (N, \zeta) \in T^*(M)\), where \(N\) is the inward-pointing unit normal to the boundary and \(\zeta \in T^*(\partial M)\) is a cotangent vector on the boundary. Consider the restriction \(W_0\) of the vector bundle \(V\) to the boundary. Let us define restrictions of the leading symbols of the operators \(R\) and \(\Delta\) to the boundary, i.e.

\[
\Pi \equiv \sigma_L(\Delta; N)|_{\partial M},
\]
\[
\nu \equiv \sigma_L(R; N)|_{\partial M},
\]
\[
\mu \equiv \sigma_L(R; \zeta)|_{\partial M}.
\]

From Eq. (32) we have thus the identity

\[
\Pi \nu = 0,
\]

Moreover, from (33) and (34) we have also

\[
\bar{\nu}\nu = I_G,
\]
\[
\bar{\nu}\mu + \bar{\mu}\nu = 0,
\]
\[
\bar{\mu}\mu = |\zeta|^2 I_G,
\]
\[
\Pi = I_\nu - \nu \bar{\nu}.
\]

From (42) and (43) we find that \(\Pi : W_0 \rightarrow W_0\) is a self-adjoint projector orthogonal to \(\nu\),

\[
\Pi^2 = \Pi, \quad \Pi \nu = 0, \quad \bar{\Pi} = \Pi.
\]

Then, a part of the boundary conditions for the operator \(F\) reads

\[
\Pi \varphi|_{\partial M} = 0.
\]

The gauge transformation of this equation is

\[
\Pi R\epsilon|_{\partial M} = 0.
\]
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The normal derivative does not contribute to this equation, and hence, if Dirichlet boundary conditions are imposed on $\epsilon$,

$$\epsilon \Big|_{\partial M} = 0,$$

the equation (49) is identically satisfied.

The easiest way to get the other part of the boundary conditions is just to set

$$\bar{R}\phi \Big|_{\partial M} = 0.$$  \hspace{1cm} (51)

Bearing in mind eq. (5) we find that, under the gauge transformations (1), this is transformed into

$$L\epsilon \Big|_{\partial M} = 0.$$  \hspace{1cm} (52)

If some $\epsilon$ is a zero-mode of the operator $L$, i.e. $\epsilon \in \text{Ker}\, L$, this is identically zero. For all $\epsilon \notin \text{Ker}\, L$ this identically vanishes when the Dirichlet boundary conditions (50) are imposed. In other words, the requirement of gauge invariance of the boundary conditions (36) determines in an almost unique way (up to zero-modes) that the ghost boundary operator $B_L$ should be of Dirichlet type. Anyway, Dirichlet boundary conditions for the operator $L$ are sufficient to achieve gauge invariance of the boundary conditions for the operator $F$.

Since the operator $\bar{R}$ in the boundary conditions (51) is a first-order operator, the set of boundary conditions (48) and (51) follows the general scheme formulated in Ref. [1]. Separating the normal derivative in the operator $\bar{R}$ we find exactly the Gilkey–Smith boundary conditions [2] for operators of Laplace type:

$$\left( \begin{array}{cc} \Pi & 0 \\ \Lambda & I_V - \Pi \end{array} \right) \left( \begin{array}{c} [\phi]_{\partial M} \\ [\phi; N]_{\partial M} \end{array} \right) = 0,$$

where

$$\Lambda \equiv (I_V - \Pi) \left[ \frac{1}{2} \left( \Gamma^i \hat{\nabla}_i + \hat{\nabla}_i \Gamma^i \right) + S \right] (I_V - \Pi),$$

the matrices $\Gamma^i$ having the form

$$\Gamma^i = -\nu \mu^i \bar{\nu},$$

and $S$ being an endomorphism. The matrices $\Gamma^i$ are anti-self-adjoint, $\bar{\Gamma}^i = -\Gamma^i$, and satisfy the relations

$$\Pi \Gamma^i = \Gamma^i \Pi = 0.$$
Thus, one can now define the matrix

$$T \equiv \Gamma \cdot \zeta = -\nu \bar{\nu} \mu \bar{\mu},$$

(57)

where $\mu \equiv \mu^j \zeta_j$, and study the condition of strong ellipticity $|\zeta|_{I_V} - iT > 0$ obtained in Ref. [1]. Such a condition now reads

$$|\zeta|_{I_V} - iT = |\zeta|_{I_V} + i\nu \bar{\nu} \mu \bar{\mu} > 0.$$  

Moreover, using the eqs. (55), (44) and (45) we evaluate

$$\Gamma^{(i \Gamma^j)} = -(I_V - \Pi)\mu^j \bar{\mu} (I_V - \Pi).$$

(59)

Therefore

$$T^2 = \Gamma^i \Gamma^j \zeta_i \zeta_j = -(I_V - \Pi)\mu \bar{\mu} (I_V - \Pi),$$

(60)

and

$$T^2 + |\zeta|^2 I_V = |\zeta|^2 \Pi + (I_V - \Pi) [ |\zeta|^2 I_V - \mu \bar{\mu}] (I_V - \Pi).$$

(61)

Since for non-vanishing $\zeta$ the part proportional to $\Pi$ is positive-definite, the condition of strong ellipticity for bosonic gauge theory means

$$(I_V - \Pi) [ |\zeta|^2 I - \mu \bar{\mu}] (I_V - \Pi) > 0.$$  

(62)

We have thus proved a theorem:

Let $V$ and $G$ be two vector bundles over a compact Riemannian manifold $M$ with smooth boundary, such that $\dim V > \dim G$. Consider a bosonic gauge theory and let the first-order differential operator $R : C^\infty(G, M) \to C^\infty(V, M)$ be the generator of infinitesimal gauge transformations. Let $\Delta : C^\infty(V, M) \to C^\infty(V, M)$ be the gauge-invariant second-order differential operator of the linearized field equations. Let the operators $L \equiv \bar{R}R : C^\infty(G, M) \to C^\infty(G, M)$ and $F \equiv \Delta + R\bar{R}$ be of Laplace type and normalized by $\sigma_L(L) = |\zeta|^2 I_G$. Let $\sigma_L(R; N)|_{\partial M} \equiv \nu$ and $\sigma_L(R; \zeta)|_{\partial M} \equiv \mu$ be the restrictions of the leading symbol of the operator $R$ to the boundary, $N$ being the inward-pointing unit normal to the boundary and $\zeta \in T^* (\partial M)$ being a cotangent vector, and $\Pi = I_V - \nu \bar{\nu}$.

Then the generalized boundary-value problem $(F, B_F)$ with the boundary operator $B_F$ determined by the boundary conditions (48) and (51) is gauge-invariant provided that the ghost boundary operator $B_L$ takes the Dirichlet form. Moreover, it is strongly elliptic.
with respect to the cone $C - \mathbb{R}_+$ if and only if the matrix $[\zeta | I_V + i\nu \bar{\mu} \bar{\nu}]$ is positive-definite. A sufficient condition for that reads

$$\left( I_V - \Pi \right) [||\zeta|^2 I_V - \mu \bar{\mu}] (I_V - \Pi) > 0.$$  \hfill (63)

In Euclidean quantum gravity, however, if a gauge-averaging functional of the de Donder type is chosen, with a gauge parameter such that the resulting operator on metric perturbations is of Laplace type, the boundary-value problem with boundary conditions (48) and (51) fails to be strongly elliptic [1]. Such a result raises deep interpretative issues, since it seems to imply that a Becchi–Rouet–Stora–Tyutin-invariant quantization of the gravitational field cannot be implemented on manifolds with boundary (cf. Ref. [3]). Two alternatives seem therefore to emerge:

(i) use local boundary conditions which are not completely gauge-invariant because they do not involve tangential derivatives and hence preserve strong ellipticity. The corresponding quantum amplitudes should however be gauge-invariant [4].

(ii) study non-local boundary conditions [5] and try to understand whether they are compatible with ellipticity, self-adjointness and with the request of invariance under a suitable class of transformations.

It seems therefore that we are still at the very beginning in the process of understanding the interplay between the problems of Euclidean quantum gravity on the one hand, and the problems of global analysis on the other hand (different aspects of the same problem have been discussed in Refs. [6,7]). Hopefully, new perspectives in fundamental physics and spectral geometry will be gained from such efforts.

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**Appendix**

In the presence of a boundary for a Riemannian manifold $M$ of dimension $m$, the local coordinates $x^\mu$, $(\mu = 1, \ldots, m)$, are split into local coordinates $\hat{x}^k$, $(k = 1, \ldots, m - 1)$, on $\partial M$, and the geodesic distance to the boundary, $r$. Similarly, the coordinates $\xi_\mu$ on the cotangent bundle $T^*(M)$ are split into coordinates $\zeta_k$ on $T^*(\partial M)$, jointly with a real
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parameter $\omega$. The notion of ellipticity we are interested in requires now that the leading symbol $\sigma_L(F)$ of an operator $F$ of Laplace type should be elliptic in the interior of $M$, and that a unique solution should exist of the ordinary differential equation:

$$\left[-\frac{d^2}{dr^2} + |\zeta|^2 - \lambda\right] \varphi(r) = 0,$$

subject to the boundary conditions and to a decay condition at infinity. A thorough formulation of boundary conditions needs indeed some abstract thinking. For this purpose, one has to consider two vector bundles $W_F$ and $W'_F$ over the boundary of $M$, with a boundary operator $B_F$ relating their sections, i.e.

$$B_F : C^\infty(W_F, \partial M) \to C^\infty(W'_F, \partial M).$$

All the information about normal derivatives of the fields is not encoded in $B_F$ but in the boundary data $\psi_F(\varphi) \in C^\infty(W_F, \partial M)$. In our analysis one has

$$\psi_F(\varphi) = \begin{pmatrix} [\varphi]_{\partial M} \\ [\varphi,N]_{\partial M} \end{pmatrix},$$

and the strong ellipticity conditions demands that a unique solution of Eq. (A.1) should exist, subject to the boundary condition

$$\sigma_g(B_F)\psi_F(\varphi) = \psi'_F(\varphi) \quad \forall \psi'_F(\varphi) \in C^\infty(W'_F, \partial M)$$

and to the asymptotic condition

$$\lim_{r \to \infty} \varphi(r) = 0.$$

With a standard notation, $\sigma_g(B_F)$ is the \textit{graded leading symbol} of the boundary operator $B_F$. When the boundary conditions (53) are considered, one finds

$$\sigma_g(B_F) = \begin{pmatrix} \Pi & 0 \\ iT & I_V - \Pi \end{pmatrix},$$

where $T$ is the anti-self-adjoint matrix defined in (57).

When all the above conditions are satisfied $\forall \zeta \in T^*(\partial M), \forall \lambda \in \mathbb{C} - \mathbb{R}_+, \forall (\zeta, \lambda) \neq (0,0)$, the boundary-value problem $(F, B_F)$ is said to be strongly elliptic with respect to the cone $\mathbb{C} - \mathbb{R}_+$. This property is crucial to ensure the existence of the asymptotic expansion as $t \to 0^+$ of the $L^2$-trace, $\text{Tr}_{L^2} \exp(-tF)$, which is frequently applied in quantum field theory and spectral geometry.
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