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BOUNDARY CONDITIONS FOR QUANTUM COSMOLOGY

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Quantum field theory can be formulated as a path integral over field configurations between initial and final surfaces. This is the approach which is usually adopted, for example in quantum cosmology. This raises the question as to which suitable boundary conditions have to be imposed for various types of field. We answer this question and calculate the one-loop corrections to the wave function of the universe.

1. Introduction

In the Casimir effect, two uncharged conducting surfaces with a narrow gap between them are seen to be attracted towards one another. The explanation of this effect lies in the way in which quantum fields respond to the presence of boundaries. A free field can be decomposed into a collection of oscillators whose frequencies depend on the size and shape of the boundary and the type of boundary conditions [1].

The same features arise in the calculation of transition amplitudes between field configurations using the Feynman sum over histories, in this case the fields being fixed on initial and final hypersurfaces. Transition amplitudes calculated this way are particularly useful in investigating a wide range of non-perturbative phenomena. They can also be useful in situations where a scattering matrix cannot be defined, which means that they are of considerable importance in quantum cosmology for calculations involving the wave function of the Universe [2].

Some information about these quantum processes can be obtained from the asymptotic expansion of a heat kernel. Individual terms in the expansion are associated with quantum divergences and the rescaling behaviour of transition amplitudes or effective potentials [3]. Recently, the relevant term for the rescaling properties of four-dimensional field theories with boundaries has been obtained [4–6]. This result enables us to examine the one-loop corrections to quantum phenomena for general fields on arbitrary backgrounds.

Before discussing the effects of boundaries we have to decide upon suitable boundary conditions. The type of boundary conditions which are used depends

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upon the physical situation under investigation. This paper will be mainly concerned with the evaluation of transition amplitudes between different field configurations. It is important to realise that it would often be incorrect to fix all of the field components. For fermionic fields this would be an overdetermined problem leading to a vanishing amplitude. Only half of the field components should be specified, which can be done using projection operators $P_{\pm}$ [7, 8]. The forms of these projection operators is fixed by self-adjointness of the Dirac operator. This condition is most important as it guarantees that the fields can be decomposed into eigenmodes with a real spectrum of frequencies.

With gauge fields it is necessary to fix the gauge freedom and introduce ghost fields. The gauge independence of the theory depends on a residual BRS symmetry and this can be used to relate the boundary conditions of the gauge and ghost fields. Together with a self-adjointness condition on the respective wave operators, this is enough to determine the form which the boundary conditions must take for a given gauge-fixing term. These are a mixture of conditions which fix the fields and conditions which fix the normal derivatives. The same also applies to the gravitational field. The intrinsic geometry of the boundary has to be fixed, but the normal components of the metric on the boundary are free. Instead, there are restrictions upon the normal derivatives of the metric perturbations.

These boundary conditions are the ones relevant for the path integral approach to quantum cosmology. In sect. 3 we have analysed a wave function for the universe in a simple model which includes a scalar matter field. Under the assumption that the universe has no initial boundary, it is possible to find the approximate behaviour of the wave function for large values of the scalar field, using the scaling properties of the path integral. Quantum corrections to the wave function have been considered before for small values of the radius [10, 11, 19], but our results are more general and our treatment of the gauge fields is more complete.

If we adopt the view point that the square of the wave function represents a probability distribution, then the likelihood of different initial values of the scalar field can be compared. In the absence of quantum corrections, the wave function predicts a uniform distribution of large values. The quantum corrections drive this distribution to zero or to infinity at energies beyond the Planck scale depending on the particle content. This result agrees with Barvinsky and Kamenshchik [13], although the forms of the expressions found by us disagree substantially with these authors.

2. Boundary conditions for transition amplitudes

The transition amplitude between field configurations ϕ_1 and ϕ_2 on initial and final surfaces Σ_1 and Σ_2 can be defined by a path integral over field configurations

TABLE 1

Field	Operator	$\Im$
scalar	$-\nabla^2+(\zeta+\frac{1}{6})R+m^2$	
ghost	$-\nabla^2$	
spinor	$\gamma\cdot\nabla+m$	
Maxwell	$-\delta_a{}^b\nabla^2+R_a{}^b$	$\nabla\cdot A$
ghost	$-\delta_a{}^b\nabla^2-R_a{}^b$	
graviton	$\delta_{ab}{}^{cd}(-\nabla^2+R-2\Lambda)-2R_{ab}{}^{cd}-2R_a{}^c\delta_b{}^d$	$\nabla^a\bar{h}_{ab}$

which interpolate between them. We shall write the amplitude as

$$\mathrm{e}^{-\Gamma(\phi_1,\phi_2)}=\int \mathrm{d}\mu\,[\phi]\mathrm{e}^{-S[\phi]},$$

where $S[\phi]$ is the euclidean action.

In the semiclassical approximation the path integral is dominated by saddle point paths ϕ_S which satisfy the classical equations $\delta S=0$ and agree with the boundary data on Σ_1 and Σ_2 [3]. The fields can be expanded about these saddle points to obtain a perturbative expansion of the transition amplitudes,

$$\Gamma=\Gamma^{(0)}+\Gamma^{(1)}+\dots,$$

with leading-order term $\Gamma^{(0)}=S[\phi_S]$. The one-loop term involves a linear operator A in a background field ϕ_S,

$$\Gamma^{(1)}=\tfrac{1}{2}\log\det A\,.$$

In order to simplify our discussion we will only consider constant background fields. Then the wave operator separates into the different forms given in table 1, for different types of field [8].

Gauge fields can only correctly be accounted for if we introduce gauge-fixing terms $\Im[\phi]$ and corresponding ghost fields. The operators tabulated in table 1 are associated with the gauge-fixing terms given in the final column. Then

$$\Gamma^{(1)}=\tfrac{1}{2}\sum_j(-1)^{f_j}\log\det A_j,$$

where j labels the different types of field and $f_j=1$ for fermions or ghosts. Complex fields, including ghost fields, are counted as two fields in this expression.

So far, the relationship between the fields given on the boundary and the interior fields has not been defined precisely. For fermion fields it would not be appropriate to fix all of the field components on the boundary because this would overspecify the eigenvalue problem for the Dirac operator. Instead, we fix a subset of fields $P\psi$, defined by a projection operator P. Therefore, the boundary conditions on the classical fields ψ_S are

$$P\psi_S = \psi_1$$

and the fluctuations $\hat{\psi}$ satisfy

$$P\hat{\psi} = 0 .$$

With these boundary conditions the Dirac operator can be self-adjoint only if P has the form [7]

$$P = \mathrm{e}^{\alpha\gamma_5} P_- \, \mathrm{e}^{-\alpha\gamma_5} ,$$

where

$$P_- = \tfrac{1}{2}(1 - \gamma_5 \gamma \cdot n) .$$

We shall take $P = P_-$. This is the only choice of projection operator which commutes with charge conjugation and can be applied to both Majorana and Dirac spinors.

Self-adjointness of the Dirac operator $\gamma \cdot D$ can be used to find out more about the behaviour of $\hat{\psi}$ near to the boundary. Since the operator must act as a mapping on the subspace defined by the projection operators, we have

$$P_+ \gamma \cdot D P_- = 0 .$$

From this it can be shown that [9]

$$\left(\tfrac{1}{2}k + n \cdot D\right) P_+ \hat{\psi} = 0, \qquad P_- \hat{\psi} = 0 ,$$

where k is the intrinsic curvature of the boundary. Used together, these conditions determine eigenstates of $(\gamma \cdot D)^2$ and we can make use of the relationship

$$\log\det \gamma \cdot D = \tfrac{1}{2} \log\det(\gamma \cdot D)^2$$

in evaluating $\Gamma^{(1)}$.

Boundary conditions on the gauge fields A are related to those of the ghost fields η and $\bar{\eta}$ because of BRS invariance,

$$\delta A^a = \bar{\epsilon} \nabla^a \eta , \qquad \delta\eta = 0, \qquad \delta\bar{\eta} = \bar{\epsilon} \Im .$$

This symmetry ensures that the transition amplitudes do not depend on the choice of gauge or gauge-fixing term. For the operators given in table 1 there are two choices of boundary condition for which the ghost operator is self-adjoint, Dirichlet or Neumann. Consider the Neumann condition on the ghost perturbation $\hat{\eta}$,

$$n \cdot \nabla \hat{\eta} = 0 .$$

This implies that we can fix the normal component of A on the boundary consistently with the BRS symmetry, but the other components of A change under a BRS transformation. The only mixed boundary conditions for perturbations $\hat{A}$ which are preserved under the BRS symmetry are

$$n \cdot \hat{A} = 0, \qquad \left(k_a^b + \delta_a{}^b n \cdot \nabla\right) P \hat{A} = 0 ,$$

where P is the tangential projection operator $\delta_a{}^b - n_a n^b$. The latter equation is the statement that the electric field vanishes on the boundary.

When the ghost satisfies Dirichlet boundary conditions then the tangential components of the gauge field are unchanged by a BRS transformation and can be fixed. This corresponds to fixing the magnetic field on the boundary. The surface divergence of the field $\hat{A}$, which can be written

$$(P\nabla) \cdot (P\hat{A}) = \Im - (k + n \cdot \nabla) n \cdot \hat{A} ,$$

must also vanish. We see from the BRS transformations that $\Im$ is zero on the boundary, and therefore the mixed boundary conditions in this case take the form

$$P\hat{A} = 0, \qquad (k + n \cdot \nabla) n \cdot \hat{A} = 0 .$$

These boundary conditions are also the appropriate ones to use at the surface of a conducting body with normal vector n. They imply that the normal component of the magnetic field and the tangential components of the electric field vanish.

These results can be extended to non-abelian gauge theories without any difficulty. We first expand the gauge fields about a background A_s and introduce a gauge-fixing term $\Im(A_s, \hat{A})$. The path integral should then be invariant under a gauge symmetry of the background fields and a BRS symmetry. Together these ensure that the results do not depend upon the choice of gauge or gauge-fixing term and they can be used to derive Ward identities. The BRS transformations are

$$\delta A_s = 0, \qquad \delta \hat{A} = \epsilon D\left[A_s + \hat{A}\right] \eta ,$$

$$\delta \eta = -\epsilon \tfrac{1}{2} [\eta, \eta], \qquad \delta \bar{\eta} = \epsilon \Im .$$

As before there are electric and magnetic boundary conditions. In the magnetic case, with Dirichlet boundary conditions on the ghost,

$$P\hat{A}=0, \qquad (k+n\cdot D[A_s])n\cdot\hat{A}=0,$$

for $\Im=D_a[A_s]\hat{A}^a$.

Similar considerations can be used to find suitable boundary conditions for the metric fluctuations h_{ab} and the gravity ghost $\hat{\epsilon}_a$. The BRS transformations are

$$\delta h_{ab}=2\nabla_{(a}\epsilon_{b)}, \qquad \delta\epsilon_a=0, \qquad \delta\bar{\epsilon}_a=\nabla^b\bar{h}_{ab},$$

where

$$\bar{h}_{ab}=h_{ab}-\tfrac{1}{2}g_{ab}h.$$

We shall impose Dirichlet boundary conditions on the normal components of the ghost field,

$$n\cdot\epsilon_a=0.$$

From the BRS invariance this implies that the normal component of the gauge-fixing term vanishes.

$$n^a\nabla_b\bar{h}^b{}_a=P^{ab}\nabla_b\left(n^dP_a{}^c\bar{h}_{cd}\right)+(2k+n\cdot\nabla)n^an^b\bar{h}_{ab}-(k^{ab}-kP^{ab})h_{ab}.$$

There are only two sets of boundary conditions on the metric perturbations which are consistent with this condition and self-adjointness. One of these has

$$P_a{}^cP_b{}^dh_{cd}=0, \qquad (2k+n\cdot\nabla)n^an^b\bar{h}_{ab}=0, \qquad P_a{}^cn^dh_{cd}=0.$$

The BRS invariance of the last of these conditions leads to boundary conditions on the ghost field,

$$n\cdot\epsilon=0, \qquad \left(-k_a{}^b+n\cdot\nabla\right)P_a^b\epsilon_b=0.$$

These boundary conditions correspond to fixing the intrinsic geometry of the initial and final hypersurfaces. They are not entirely BRS invariant because the surface components change under BRS transformations, but this does not affect the gauge invariance of the resulting transition amplitudes.

The boundary conditions on the metric perturbations can be written in terms of a single projection operator P_+ defined as

$$P_+=n_an_b\left(2n^cn^d-g^{cd}\right).$$

Then they take the form

$$P_- h = 0, \qquad (2k + n \cdot \nabla) P_+ h = 0,$$

which is the form that we shall use in sect. 3.

3. The trace anomaly and quantum cosmology

The effective action introduced in sect. 2 is infinite and has to be regulated. Using ζ-functions,

$$\zeta_j(s) = \sum_i \lambda_i^{-s},$$

where λ_i are eigenfunctions of the operator A_j, allows us to define [3]

$$\Gamma_j^{(1)} = -\tfrac{1}{2}\zeta_j'(0) - \tfrac{1}{2}\zeta_j(0)\log\mu^2.$$

This introduces a renormalization scale μ and β-functions can be read off the terms in $\zeta_j(0)$.

Recent results on the heat kernel expansion can be used to find $\zeta_j(0)$ on general backgrounds with arbitrary boundaries. These results are summarized in appendix A. The relevant operators can be found in table 1 and the boundary conditions are given in sect. 2. We may then use the result

$$\zeta_j(0) = B_2(j)$$

to express $\zeta_j(0)$ in terms of local invariants $b_2(j)$ and surface terms $c_2(j)$.

We shall restrict attention to gravitational backgrounds which satisfy

$$R_{ab} = \Lambda g_{ab}$$

and constant scalar field backgrounds. The results may then be expressed as

$$b_4 = \alpha_0 \Lambda^2 + \alpha_1 R_{abcd} R^{abcd}$$

and

$$c_4 = \beta_1 \Lambda k + \beta_2 k^3 + \beta_3 k k_{ab} k^{ab} + \beta_4 k_a^b k_b^c k_c^a + \beta_5 C_{abcd} k^{ac} n^b n^d.$$

The values of α and β are tabulated in table 2. In this table the ghost contributions have been combined with their respective gauge fields and mass terms have been set to zero. The volume terms agree with the results of Christensen et al. [14].

The use of these results is best illustrated by an example. We shall examine the Hartle–Hawking wave function of the universe [2] for a scale factor a and a homogeneous scalar field ϕ. The situation where ϕ is large and a is small is

TABLE 2

Spin	α_0	α_1	β_1	β_2	β_3	β_4	β_5
0	$8\zeta^2 - \frac{1}{45}$	$\frac{1}{180}$	$-\frac{4}{3}\zeta - \frac{1}{135}$	$\frac{1}{189}$	$-\frac{11}{315}$	$\frac{8}{189}$	$\frac{2}{45}$
$\frac{1}{2}$	$\frac{2}{15}$	$-\frac{7}{360}$	$\frac{41}{135}$	$\frac{17}{945}$	$-\frac{92}{315}$	$\frac{199}{945}$	$\frac{23}{45}$
1	$-\frac{4}{15}$	$-\frac{13}{180}$	$-\frac{2}{135}$	$-\frac{338}{945}$	$\frac{16}{63}$	$\frac{194}{945}$	$\frac{34}{45}$
2	$-\frac{2088}{180}$	$\frac{212}{180}$	$-\frac{602}{135}$	$-\frac{956}{135}$	$\frac{1652}{315}$	$\frac{56}{135}$	$\frac{64}{45}$

relevant for the inflationary scenario of the early universe, and we shall restrict our attention to this case. We shall obtain the one-loop correction to the wave function by relating this to the trace anomaly. Other authors have used the trace anomaly in quantum cosmology as a source for the classical field equations [12], but as this mixes different orders in perturbation theory we do not wish to do this here. The arguments below are very similar to those of Barvinsky and Kamenshchik [13] but our results are completely different.

The wave function is defined by a path integral as before but with a single boundary surface Σ on which the geometry is specified. The fields can be expanded about a classical background which satisfies the Einstein equations with the given boundary fields and then

$$\psi(a,\phi) = \mathrm{e}^{-\Gamma^{(0)}-\Gamma^{(1)}}$$

to one-loop order.

For sufficiently large ϕ the time variation of ϕ_j can be ignored and the field only enters the equations through a potential term $V(\phi)$ which acts as a cosmological constant $\Lambda = 8\pi G V(\phi)$ [15]. The equations can be solved by a four-sphere of radius $\bar{a}$ given by

$$\bar{a}(\phi)^2 = \frac{3}{8\pi G V(\phi)}\,.$$

For $a < \bar{a}$ the boundary conditions can be satisfied by taking part of the four-sphere as shown in fig. 1. The classical action is then

$$\Gamma^{(0)} = -\pi\bar{a}^2 f(a/\bar{a})\,,$$

where

$$f(x) = \tfrac{1}{2} - \tfrac{1}{2}(1-x^2)^{3/2}\,.$$

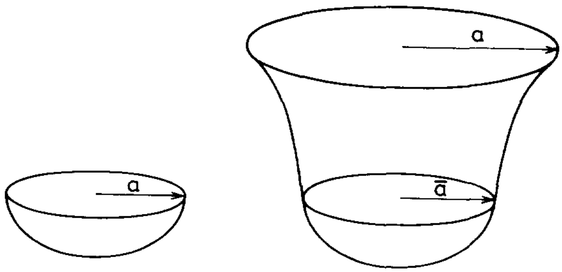

Fig. 1.

The one-loop contribution to the wave function can be found by a rescaling argument. Apart from mass terms, all of the operators in table 1 rescale under constant scaling of the four-sphere. If $\bar{a} \to \lambda \bar{a}$ then $A_j \to \lambda^{-2} A_j$. We shall consider fields whose mass $m_j \ll \bar{a}^{-1}$. Keeping $a/\bar{a}$ fixed, we deduce that

$$\Gamma_j^{(1)}(\bar{a}) = \Gamma_j^{(1)}(\bar{a}_0) - \tfrac{1}{2} B_2(j) \log(\bar{a}/\bar{a}_0)^2 .$$

Consequently

$$\mathrm{e}^{-\Gamma^{(1)}(\bar{a})} = \mathrm{e}^{-\Gamma^{(1)}(\bar{a}_0)} \left(\frac{\bar{a}}{\bar{a}_0} \right)^{\Sigma_j (-1)^{f(j)} B_2(j)} .$$

We can now use the results in table 2 to find $B_2(j)$. These take the form

$$B_2 = \gamma_1 + \gamma_2 (1 - a^2/\bar{a}^2)^{1/2} + \gamma_3 (1 - a^2/\bar{a}^2)^{3/2} ,$$

where the coefficients are given in table 3.

TABLE 3

Spin	γ_1	γ_2	γ_3
0	$6\zeta^2 - \frac{1}{180}$	$-9\zeta^2 - \frac{3}{2}\zeta$	$3\zeta^2 + \frac{3}{2}\zeta$
$\frac{1}{2}$	$\frac{11}{180}$	$\frac{1}{4}$	$-\frac{1}{2}$
1	$-\frac{31}{90}$	$\frac{1}{2}$	-1
2	$-\frac{571}{90}$	$\frac{9}{2}$	$-\frac{65}{4}$

So far we have restricted our attention to the case $a < \bar{a}$. For $a > \bar{a}$ the background solutions are generally complex, but they can be identified with hemispheres joined to de Sitter space along a maximal slice, as shown in fig. 1 [16]. This slice represents a change from imaginary time to real time, and is arguably the point at which it makes sense to think of a classical universe. The wave function there can be used to define a probability distribution on the set of different initial conditions for the scalar field by taking the modulus squared, thus

$$P(\bar{a}(\phi),\phi) = P(\bar{a}(\phi_0),\phi_0)\left(\frac{\bar{a}(\phi)}{\bar{a}(\phi_0)}\right)^{2\sum_j(-1)^{f(j)}B_2(j)} \mathrm{e}^{-\pi\bar{a}^2(\phi)+\pi\bar{a}^2(\phi_0)}.$$

This result has a familiar form. The exponential term is the nucleation probability of the universe which was obtained in ref. [17] using the theory of false vacuum decay and the exponent is the action of the gravitational instanton first introduced in that context.

For very large ϕ the exponential term in the probability approaches a constant. This is also the regime where the Einstein theory probably breaks down. According to the result, the universe emerges from below or above the Planck length depending upon the sign of $\zeta(0)$. From table 3 we see that, for $\zeta = 0$,

$$\sum_j (-1)^{f(j)} B_2(j) = -\tfrac{571}{90} - \tfrac{11}{180}N_{1/2} - \tfrac{31}{90}N_1 - \tfrac{1}{180}N_0\,,$$

where N_j is the number of real fields of spin j. It therefore appears that the probability grows with increasing energy scale and the nucleation of the universe is pushed towards the Planck scale.

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Appendix A

We shall summarise some recent results on the heat kernel expansion of an operator on a manifold with boundary. The integrated heat kernel is defined in terms of the eigenvalues by

$$K(t) = \sum_i \mathrm{e}^{-\lambda_i t}.$$

This function has an asymptotic expansion for small t of the form

$$K(t) \sim t^{-2} \sum_n B_n t^n\,,$$

where it is known that the coefficients B_n can be expressed as integrals of local invariants [18],

$$16\pi^2 B_n = \int_{\mathrm{M}} b_n \,\mathrm{d}\mu + \int_{\partial\mathrm{M}} c_n \,\mathrm{d}\mu .$$

Consider the scalar operator

$$-D^2 + X ,$$

where D_a is a gauge derivative. The volume terms up to b_3 have been known for some time. Explicitly,

$$b_2 = \mathrm{tr}\left(\tfrac{1}{72}R^2 - \tfrac{1}{180}R^{ab}R_{ab} + \tfrac{1}{180}R^{abcd}R_{abcd} - \tfrac{1}{6}RX + \tfrac{1}{2}X^2 + \tfrac{1}{12}F^{ab}F_{ab}\right),$$

where R_{abcd} is the Riemann tensor and F_{ab} is the gauge field strength [18]. Fields with spins other than zero can be handled using a tetrad formalism, where the indices on the field are thought of as internal indices with a gauge group of rotations.

The surface terms depend upon the choice of boundary conditions. We have used mixtures of Dirichlet and Neumann boundary conditions,

$$P_-\phi = 0, \qquad (\psi + n\cdot\nabla)P_+\phi = 0 ,$$

where $P_\pm$ are projection operators. Following ref. [5] we shall express the results in terms of polynomials,

$$q = \tfrac{8}{3}k^3 + \tfrac{16}{3}k_a^b k_b^c k_c^a - 8kk_{ab}k^{ab} + 4kR - 8R_{ab}(kn^a n^b + k^{ab}) + 8R_{abcd}k^{ac}n^b n^d$$

and

$$g = k_a^b k_b^c k_c^a - kk_{ab}k^{ab} + \tfrac{2}{9}k^3 .$$

For Dirichlet boundary conditions

$$c_2^{\mathrm{D}} = -\tfrac{1}{360}q + \tfrac{2}{35}g - \tfrac{1}{3}\left(X - \tfrac{1}{6}R\right)k - \tfrac{1}{2}n\cdot\nabla\left(X - \tfrac{1}{6}R\right) + \tfrac{1}{15}C_{abcd}n^b n^d k^{ac} ,$$

whilst for Robin boundary conditions

$$c_2^{\mathrm{R}} = -\tfrac{1}{360}q + \tfrac{2}{45}g - \tfrac{1}{3}\left(X - \tfrac{1}{6}R\right)k + \tfrac{1}{2}n\cdot\nabla\left(X - \tfrac{1}{6}R\right) - \tfrac{4}{3}\left(\psi - \tfrac{1}{3}k\right)^3$$
$$+ 2\left(X - \tfrac{1}{6}R\right)\psi + \left(\psi - \tfrac{1}{3}k\right)\left(\tfrac{2}{45}k^2 - \tfrac{2}{15}k_{ab}k^{ab}\right) + \tfrac{1}{15}C_{abcd}n^b n^d k^{ac} .$$

The final term in each of these expressions was missing in ref. [4] and introduced in ref. [5]. For mixed boundary conditions,

$$c_2 = \mathrm{tr}\Big(P_+ c_2^{\mathrm{R}} + P_- c_2^{\mathrm{D}} - \tfrac{7}{15} P_{+|a} P_+{}^{|a} k + \tfrac{1}{15} P_{+|a} P_{+|b} k^{ab} + \tfrac{4}{3} P_{+|a} P_+{}^{|a} P_+ \psi + \tfrac{2}{3} P_+ P_+{}^{|a} n^b F_{ab} \Big),$$

where $P_{+|a}$ denotes the surface derivative of P_+. This expression contains two terms from Branson and Gilkey [6] which were also missing in ref. [4]

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