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Review

DeWitt Boundary Condition in One-Loop Quantum Cosmology

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Abstract: DeWitt's suggestion that the wave function of the universe should vanish at the classical Big Bang singularity is considered here within the framework of one-loop quantum cosmology. For pure gravity at one loop about a flat four-dimensional background bounded by a 3-sphere, three choices of boundary conditions are considered: vanishing of the linearized magnetic curvature when only transverse-traceless gravitational modes are quantized; a one-parameter family of mixed boundary conditions for gravitational and ghost modes; and diffeomorphism-invariant boundary conditions for metric perturbations and ghost modes. A positive $\zeta(0)$ value in these cases ensures that, when the three-sphere boundary approaches zero, the resulting one-loop wave function approaches zero. This property may be interpreted by saying that, in the limit of small three-geometry, the resulting one-loop wave function describes a singularity-free universe. This property holds for one-loop functional integrals, which are not necessarily equivalent to solutions of the quantum constraint equations.

Keywords: quantum cosmology; boundary conditions; strong ellipticity; spectral ζ-function

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1. Introduction

After the birth of relativistic cosmology thanks to Friedmann's work [1], and the subsequent proof of the singularity theorems of Penrose, Hawking, and Geroch [2–7], it became well-accepted by the scientific community that classical general relativity leads to the occurrence of cosmological singularities (a spacetime being singular if it is timelike or null geodesically incomplete) in a generic way. Since then, several developments occurred, and in particular, we here mention what follows.

(i) At the classical level, the work of Christodoulou and Klainerman [8] led to the discovery of asymptotically flat spacetimes, which are timelike geodesically complete.
(ii) At the quantum level, DeWitt [9] proposed to look at the behavior of the wave function of the universe in correspondence with the classical Big Bang singularity. Such a proposal was assessed in the outstanding work in Ref. [10].
(iii) Over many years, various concepts of singularity have been conceived, as can be seen in an important review of Kamenshchik [11].

Moreover, in the literature on quantum gravity and quantum cosmology, several approaches were developed to study the possible quantum origin of spacetime geometry. One-loop effects in the early universe were investigated in detail, especially with the help of ζ-function methods. It is the aim of our review to describe them and then discuss their relevance for the singularity issue in cosmology. The structure of the paper is as follows.

Section 2 presents in detail a $\zeta(0)$ calculation when only transverse-traceless perturbations are considered, with boundary conditions requiring the vanishing of linearized magnetic curvature on the three-sphere boundary. Section 3 discusses a one-parameter family of $\zeta(0)$ values obtained with mixed boundary conditions for metric perturbations and ghost fields. Sections 4–7 outline the basic steps of the $\zeta(0)$ calculation with diffeomorphism-invariant boundary conditions. Open problems are discussed in Section 8.

2. Linearized Magnetic Curvature Vanishing on S^3

We study pure gravity at one loop about flat Euclidean four-space with a three-sphere boundary of radius a, because when $a \to 0$, this is the limiting case of a four-sphere geometry bounded by a three-sphere [12]. The prefactor of the semiclassical wave function is given by the following (with I_2 denoting the part of the action quadratic in metric perturbations)

$$P(a) = \int e^{-I_2[\gamma]} \, D\gamma, \tag{1}$$

which is a functional integral over all metric perturbations γ_{ab} that are regular at the origin $\tau = 0$ and satisfy a given boundary condition at $\tau = a$. Integration is here restricted to the physical degrees of freedom, which are found by using the Hamiltonian formulation with the following transverse-traceless choice of gauge condition:

$$\sum_i (D^i \gamma)_{ij} = 0, \; \sum_k \gamma^k_k = 0. \tag{2}$$

These relations pick out the transverse-traceless tensor hyperspherical harmonics $G^{(n)}_{ij}(\phi^k)$ multiplied by functions of the radial coordinate τ. Hence, we write

$$\gamma_{ij} = \gamma^{TT}_{ij} = \sum_{n=3}^{\infty} q^n(\tau) G^{(n)}_{ij}(\phi^k). \tag{3}$$

Our work in Ref. [13] studied the Breitenlohner–Freedman–Hawking [14,15] local boundary conditions for fields of spin $0, \frac{1}{2}, 1, \frac{3}{2}, 2$. For gravity, these imply that the linearized magnetic curvature should vanish at the boundary. Our detailed analysis in Section 7.3 of Ref. [13] never appeared in any journals, and hence it is of interest to our review article.

The action that is quadratic in metric perturbations involves a second-order elliptic operator A with eigenvalues λ_n, for which one can define a spectral ζ-function

$$\zeta_A(s) = \mathrm{Tr}_{L^2} A^{-s} = \sum_n (\lambda_n)^{-s}. \tag{4}$$

Eventually, as was shown by Schleich [12], the prefactor of the semiclassical wave function of Equation (1), with γ having the form (3), can be expressed as

$$P(a) = \frac{1}{\sqrt{\det\left(\frac{-\nabla_f \nabla^f}{4\pi l_P^2 \mu^2}\right)}} = D\, a^{\zeta(0)}, \tag{5}$$

where $-\nabla_f \nabla^f$ is the Laplacian acting on transverse-traceless metric perturbations, and $\zeta(0)$ is the value at $s = 0$ of the analytic continuation of the spectral ζ-function (4) (for further details, see now the Appendix A on the one-loop approximation). Thus, within a functional-integral framework, the wave function of the universe may fulfill the DeWitt boundary condition if and only if $\zeta(0)$ is positive.

The linearized magnetic curvature for gravity is defined from the Weyl tensor C and from the normal n to the boundary according to the rule (with summation over repeated tensor indices)

$$B_{ij} \equiv \frac{1}{2} \varepsilon_{j\mu}{}^{kl} C_{kli\nu} n^\mu n^\nu,$$

and it can only vanish on S^3 if [13]

$$\sum_{n=3}^{\infty} \frac{dq^n}{d\tau}(a) \epsilon_j{}^{kl} \left(G^{(n)}_{il|k} - G^{(n)}_{ik|l} \right) = 0. \tag{6}$$

The only condition on the modes that ensures the validity of (6) is

$$\frac{dq^n}{d\tau}(a) = 0, \ \forall n \geq 3. \tag{7}$$

We are now interested in evaluating $\zeta(0)$ using (7). Thus, after setting $\tau = t$, we study the kernel of the heat equation for the operator

$$P_n \equiv -\left(\frac{d^2}{dt^2} - \frac{1}{t}\frac{d}{dt} - \frac{(n^2-1)}{t^2}\right), \ \forall n \geq 3, \tag{8}$$

which results from studying the Laplacian on transverse-traceless metric perturbations. On denoting by $E > 0$ the eigenvalues of P_n, we find that its eigenfunctions regular at the origin are (up to a multiplicative constant)

$$u_n(t) = tJ_n(\sqrt{E}t) = q^n(t). \tag{9}$$

Thus, the boundary condition (7) implies the eigenvalue condition

$$J_n(\sqrt{E}a) + \sqrt{E}a\dot{J}_n(\sqrt{E}a) = 0, \ \forall n \geq 3. \tag{10}$$

This equation is of the general kind studied in Ref. [16]. Setting now $a = 1$ for simplicity, we define the function

$$F_n(z) \equiv J_n(z) + z\dot{J}_n(z), \ \forall n \geq 3. \tag{11}$$

Of course, the consideration of such $F_n(z)$ is suggested by (10). It only has real simple zeros apart from $z = 0$ (page 482 of Ref. [17]). The basic idea is now the following [16]. Given the zeta-function at large x

$$\zeta(s, x^2) \equiv \sum_n \left(\lambda_n + x^2\right)^{-s}, \tag{12}$$

one has, in four dimensions (see Theorem 2 on page 6 of Ref. [18]),

$$\Gamma(3)\zeta(3, x^2) = \int_0^\infty t^2 e^{-x^2 t} G(t)\, dt \sim \sum_{n=0}^\infty B_n \Gamma\left(1 + \frac{n}{2}\right) x^{-n-2}, \tag{13}$$

where we have used the asymptotic expansion of the heat kernel for $t \to 0^+$, i.e.,

$$G(t) \sim \sum_{n=0}^\infty B_n t^{\frac{n}{2}-2}. \tag{14}$$

Strictly speaking, since we have not proved general results on the existence of the asymptotic expansion of the heat kernel, our Formula (14) could be initially regarded as an assumption. However, existence theorems hold for the problems studied in this paper [19,20].

On the other hand, one also has the identity

$$\Gamma(3)\zeta(3, x^2) = -\sum_{p=0}^\infty N_p \left(-\frac{1}{2x}\frac{d}{dx}\right)^3 \log\left((ix)^{-p} F_p(ix)\right), \tag{15}$$

where N_p is the degeneracy of the problem. Thus the comparison of (13) and (15) can yield the coefficients B_n and in particular $\zeta(0) = B_4$, provided we carefully perform a uniform Debye expansion of $F_p(ix)$. It should be emphasized that this technique seems to be the most efficient. In fact, by using this algorithm, Moss [16] was able to compute $\zeta(0)$ for a real scalar field subject to Robin boundary conditions, whereas the technique of Kennedy based on charge layers on the plane tangent to S^3 failed to provide such a value [21,22]. Indeed, the eigenvalue condition (10) is of the Robin type (just set $\beta = 1$ in Equation (22) of Ref. [16]). Thus, on passing to the variable $x \to ix$ and then defining $\alpha_p \equiv \sqrt{p^2 + x^2}$, $C \equiv -\log(\sqrt{2\pi})$, we can write

$$\log\Big((ix)^{-p} F_p(ix)\Big) \sim C - p\log(p + \alpha_p) + \frac{1}{2}\log(\alpha_p) + \alpha_p + \sum_{n=1}^{\infty}\sum_{r=0}^{n} a_{nr} p^{2r} \alpha_p^{-n-2r}. \quad (16)$$

The coefficients a_{nr} in (16) can be computed by comparison using the formula

$$\sum_{n=1}^{\infty}\sum_{r=0}^{n} a_{nr} t^{2r} = \sum_{m=1}^{\infty} a_m(t), \quad (17)$$

because the $a_m(t)$ values are known polynomials in t arising from uniform asymptotic expansions of Bessel functions and their first derivatives. Thus, setting $\beta = 1$ in the Formulae (29)–(31) of Ref. [16] for the $a_m(t)$, we find in our case that

$$a_{10} = \frac{5}{8},\ a_{11} = \frac{7}{24}, \quad (18)$$

$$a_{20} = -\frac{3}{16},\ a_{21} = \frac{1}{8},\ a_{22} = -\frac{7}{16}, \quad (19)$$

$$a_{30} = \frac{17}{384},\ a_{31} = \frac{389}{640},\ a_{32} = -\frac{203}{128},\ a_{33} = \frac{1463}{1152}, \quad (20)$$

plus infinitely many other coefficients that we do not strictly need here. We can now insert (16)–(20) into (15), apply three times the differential operator $-\frac{1}{2x}\frac{d}{dx}$, and finally use the contour formula for positive integer values of k [16]

$$\sum_{p=0}^{\infty} p^{2k} \alpha_p^{-2k-m} = \frac{\Gamma\left(k + \frac{1}{2}\right)\Gamma\left(\frac{m}{2} - \frac{1}{2}\right)}{2\Gamma\left(k + \frac{m}{2}\right)} x^{1-m},\ \forall k = 1, 2, 3, \ldots, \quad (21)$$

and the known properties of the Γ-function [23]. Now, writing the asymptotic expansion of the right-hand side of (15) in the form

$$\Gamma(3)\zeta(3, x^2) \sim \sum_{n=0}^{\infty} b_n x^{-n-2}, \quad (22)$$

the comparison with (15) shows that

$$\zeta(0) = B_4 = \frac{b_4}{2} = \zeta^{I}(0) + \zeta^{II}(0), \quad (23)$$

since it is well-known that the asymptotic expansion, if it exists, is unique. The two contributions to $\zeta(0)$ are obtained from the following formulae:

$$\Gamma(3)\zeta(3, x^2) \sim \Big[\sigma_1 + \sigma_2\Big] \sim \sum_{n=0}^{\infty} b_n x^{-n-2}, \quad (24)$$

$$\sigma_1 \sim -\sum_{p=0}^{\infty} N_p \left(-\frac{1}{2x}\frac{d}{dx}\right)^3 \left[-p\log(p + \alpha_p) + \frac{1}{2}\log(\alpha_p) + \alpha_p\right], \quad (25)$$

$$\sigma_2 \sim -\sum_{p=0}^{\infty} N_p \left(-\frac{1}{2x}\frac{d}{dx}\right)^3 \sum_{n=1}^{\infty}\sum_{r=0}^{n} a_{nr} p^{2r} \alpha_p^{-n-2r}. \quad (26)$$

Bearing in mind (15) and (16), we write (24)–(26) because we can apply Theorem 3 on page 7 of Ref. [18], concerning the differentiation of asymptotic expansions.

Thus, $\zeta^I(0)$ (respectively, $\zeta^{II}(0)$) is half the coefficient of x^{-6} in the asymptotic expansion of σ_1 (respectively, σ_2). We first study the asymptotic expansion of σ_2, since it is easier to perform this calculation. In our problem, the degeneracy N_p is [12]

$$N_p = 0 \; \forall p = 0, 1, 2, \;\; N_p = 2(p^2 - 4) \; \forall p \geq 3. \tag{27}$$

This is why we find

$$\sigma_2 \sim -\sum_{n=1}^{\infty} \sum_{r=0}^{n} a_{nr} \Big(r + \frac{n}{2}\Big) \Big(r + \frac{n}{2} + 1\Big) \Big(r + \frac{n}{2} + 2\Big) \Big[(G - H)(r, x, n)\Big], \tag{28}$$

where, setting $A = -8, \; B = 2$ (cf. (27)), we have, using also (21),

$$\begin{aligned} G(r, x, n) \;\; &= \;\; \sum_{p=0}^{\infty} (A + Bp^2) p^{2r} \alpha_p^{-n-2r-6} = \mathrm{O}(x^{-n-6}) \\ &+ \;\; \frac{A}{2} \frac{\Gamma\Big(r + \frac{1}{2}\Big) \Gamma\big(\frac{n}{2} + \frac{5}{2}\big)}{\Gamma\big(r + \frac{n}{2}\big)} \frac{x^{-5-n}}{\big(r + \frac{n}{2}\big)\big(r + \frac{n}{2} + 1\big)\big(r + \frac{n}{2} + 2\big)} \\ &+ \;\; \frac{B}{2} \frac{\Gamma\big(r + \frac{3}{2}\big) \Gamma\big(\frac{n}{2} + \frac{3}{2}\big)}{\Gamma\big(r + \frac{n}{2}\big)} \frac{x^{-3-n}}{\big(r + \frac{n}{2}\big)\big(r + \frac{n}{2} + 1\big)\big(r + \frac{n}{2} + 2\big)}, \end{aligned} \tag{29}$$

$$\begin{aligned} H(r, x, n) \;\; &= \;\; \sum_{p=0}^{2} 2(p^2 - 4) p^{2r} \alpha_p^{-n-2r-6} = -6x^{-n-2r-6} \left(1 + \frac{1}{x^2}\right)^{-\frac{n}{2} - r - 3} \\ &- \;\; 8\delta_{r0} x^{-n-6}. \end{aligned} \tag{30}$$

Thus, $H(r, x, n)$ gives rise to terms in (28) that contain x^{-k} with $k \geq 7$, and it does not contribute to $\zeta^{II}(0)$. This is why (28) and (29) lead to

$$\zeta^{II}(0) = \frac{1}{2} \Big[- A(a_{10} + a_{11}) - B(a_{30} + a_{31} + a_{32} + a_{33}) \Big]. \tag{31}$$

The insertion of (18), (20) and (27) into (31) finally yields

$$\zeta^{II}(0) = \frac{11}{3} - \frac{121}{360} = \frac{1199}{360}. \tag{32}$$

The calculation of (25) is more involved. By performing the three derivatives and using the identity $\frac{1}{2x} \frac{d\alpha_p}{dx} = \frac{1}{2\alpha_p}$, we find

$$\left(\frac{1}{2x} \frac{d}{dx}\right)^3 \log\left(\frac{1}{p + \alpha_p}\right) = (p + \alpha_p)^{-3} \left[-\alpha_p^{-3} - \frac{9}{8} p \alpha_p^{-4} - \frac{3}{8} p^2 \alpha_p^{-5}\right]. \tag{33}$$

This intermediate step is very important because it proves that by summing over all integer values of p from 0 to ∞, we obtain a convergent series. However, to be able to perform the $\zeta(0)$ calculation, it is convenient to use the identity

$$(p + \alpha_p)^{-3} = \frac{(\alpha_p - p)^3}{x^6}. \tag{34}$$

Upon inserting (34) into (33) and re-expressing p^2 as $\alpha_p^2 - x^2$, we obtain

$$\begin{aligned}
&\left(\frac{1}{2x}\frac{d}{dx}\right)^3\Big[-p\log(p+\alpha_p)\Big] = -px^{-6}+p^2x^{-6}\alpha_p^{-1}+\frac{p^2}{2}x^{-4}\alpha_p^{-3}+\frac{3}{8}p^2x^{-2}\alpha_p^{-5}\\
\equiv\ & M(x,\alpha_p,p),
\end{aligned} \tag{35}$$

which implies

$$\sigma_1 \sim \left[\sum_{p=0}^{\infty} N_p M(x,\alpha_p,p)\right] + \sigma_1'' \sim \Big[\sigma_1' + \sigma_1''\Big], \tag{36}$$

where

$$\begin{aligned}
\sigma_1'' &= -\sum_{p=0}^{\infty} N_p\left(-\frac{\alpha_p^{-6}}{2}-\frac{3}{8}\alpha_p^{-5}\right)\\
&= \sum_{p=0}^{\infty}(A+Bp^2)\left(\frac{\alpha_p^{-6}}{2}+\frac{3}{8}\alpha_p^{-5}\right)\\
&+ \sum_{p=0}^{2}(A+Bp^2)\left(-\frac{\alpha_p^{-6}}{2}-\frac{3}{8}\alpha_p^{-5}\right).
\end{aligned} \tag{37}$$

The infinite sum on the right-hand side of (37) contributes to $\zeta(0)$ only through the following part:

$$\sum_{p=0}^{\infty}\frac{A}{2}\alpha_p^{-6} = \frac{A}{2}\left[\frac{x^{-6}}{2}+\frac{\pi}{2}\frac{3!!}{4!!}x^{-5}\right]. \tag{38}$$

The result (38) is proved by applying the Euler–Maclaurin formula [18] to the calculation of $\sum_{p=0}^{\infty}(p^2+x^2)^{-3}$, and then using the Formula (3.249.1) on page 294 of Ref. [24]. In addition, the finite sum on the right-hand side of (37) contributes to $\zeta(0)$. In fact, one finds (we have $x \to \infty$) that

$$\begin{aligned}
&\sum_{p=0}^{2}(A+Bp^2)\left(-\frac{\alpha_p^{-6}}{2}-\frac{3}{8}\alpha_p^{-5}\right) = -\left(\frac{A}{2}+\frac{B}{2}\right)x^{-6}\left[1-\frac{3}{x^2}+\frac{6}{x^4}+...\right]\\
-\ &\frac{A}{2}x^{-6}-\frac{3}{8}Ax^{-5}\\
-\ &\frac{3}{8}(A+B)x^{-5}\left[1-\frac{5}{2x^2}+\frac{35}{8x^4}+...\right],
\end{aligned} \tag{39}$$

which implies that the total contribution of σ_1'' to $\zeta(0)$ is given by

$$\zeta^{Ib}(0) = \frac{1}{2}\left(-A-\frac{B}{2}\right)+\frac{A}{8} = \frac{7}{2}-1 = \frac{5}{2}. \tag{40}$$

Thus, we have so far

$$\zeta(0) = \zeta^{I}(0)+\zeta^{II}(0) = \zeta^{Ia}(0)+\zeta^{Ib}(0)+\zeta^{II}(0), \tag{41}$$

where

$$\zeta^{Ib}(0)+\zeta^{II}(0) = \frac{5}{2}+\frac{1199}{360}. \tag{42}$$

It now remains to compute $\zeta^{Ia}(0)$, i.e., the contribution to $\zeta(0)$ due to σ_1' in (36). Indeed, one has

$$\sigma_1' \sim \left[A\sum_{p=0}^{\infty}M(x,\alpha_p,p)+B\sum_{p=0}^{\infty}p^2M(x,\alpha_p,p)-\sum_{p=0}^{2}(A+Bp^2)M(x,\alpha_p,p)\right]. \tag{43}$$

Let us now denote by $\Sigma^{(a)}$, $\Sigma^{(b)}$ and $\Sigma^{(c)}$ the three sums on the right-hand side of (43). Both $\Sigma^{(a)}$ and $\Sigma^{(b)}$ contain divergent parts in view of (35). These fictitious divergences may be regularized by dividing by α_p^{2s} and then taking the limit as s tends to zero, as shown in Ref. [16]. It might not appear a priori obvious that this technique leads to unambiguous results, since the limit $s \rightarrow 0$ is a delicate mathematical point. However, a fundamental consistency check is presented in Section 7.4 of Ref. [13] for all one-loop calculations involving only physical degrees of freedom of bosonic fields, showing that the method is correct. In performing the calculation, we must use the contour Formula (21) and also the following asymptotic expansion [16]:

$$\sum_{p=0}^{\infty} p\alpha_p^{-1-n} \sim \frac{x^{1-n}}{\sqrt{\pi}} \sum_{r=0}^{\infty} \frac{2^r}{r!} \widetilde{B}_r x^{-r} \frac{\Gamma\left(\frac{r}{2}+\frac{1}{2}\right)\Gamma\left(\frac{n}{2}-\frac{1}{2}+\frac{r}{2}\right)}{2\Gamma\left(\frac{1}{2}+\frac{n}{2}\right)} \cos\left(\frac{r\pi}{2}\right), \tag{44}$$

where $\widetilde{B}_0 = 1$, $\widetilde{B}_1 = -\frac{1}{2}$, $\widetilde{B}_2 = \frac{1}{6}$, $\widetilde{B}_4 = -\frac{1}{30}$ etc., are Bernoulli numbers. Thus, using the label R for the regularized quantities, we define

$$\begin{aligned} \Sigma_R^{(a)} \equiv\; & A\Bigg[-x^{-6}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p\alpha_p^{-1-(2s-1)}\right) + x^{-6}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^2\alpha_p^{-2-(2s-1)}\right) \\ & + \frac{x^{-4}}{2}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^2\alpha_p^{-2-(2s+1)}\right) + \frac{3}{8}x^{-2}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^2\alpha_p^{-2-(2s+3)}\right)\Bigg]. \end{aligned} \tag{45}$$

In view of (44), the first limit in (45) gives the following contribution to $\zeta(0)$:

$$\delta_1 = -\frac{A}{2}\left(-\frac{\widetilde{B}_2}{\sqrt{\pi}}\Gamma\left(\frac{3}{2}\right)\right) = \frac{A}{24} = -\frac{1}{3}, \tag{46}$$

whereas the other limits in (45) do not contribute to $\zeta(0)$ in view of (21), because one only obtains terms proportional to x^{-4}.

Moreover, bearing in mind the identity

$$\sum_{p=0}^{\infty} p^3\alpha_p^{-2s} = \sum_{p=0}^{\infty} p\alpha_p^{-1-(2s-3)} - x^2\sum_{p=0}^{\infty} p\alpha_p^{-1-(2s-1)}, \tag{47}$$

we also define

$$\begin{aligned} \Sigma_R^{(b)} \equiv\; & B\Bigg[-x^{-6}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^3\alpha_p^{-2s}\right) + x^{-6}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^4\alpha_p^{-4-(2s-3)}\right) \\ & + \frac{x^{-4}}{2}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^4\alpha_p^{-4-(2s-1)}\right) + \frac{3}{8}x^{-2}\left(\lim_{s\to 0}\sum_{p=0}^{\infty} p^4\alpha_p^{-4-(2s+1)}\right)\Bigg]. \end{aligned} \tag{48}$$

In view of (44) and (47), the first limit in (48) gives the following contribution to $\zeta(0)$:

$$\delta_2 = -\frac{B}{2}\left(-\frac{\widetilde{B}_4}{4}\right) = -\frac{B}{240} = -\frac{1}{120}. \tag{49}$$

Note that the second sum in (47) does not contribute to δ_2 because its only constant term contains $\frac{\Gamma(s+1)}{\Gamma(s)}$, which tends to 0 as $s \rightarrow 0$. The other limits in (48) do not contribute to $\zeta(0)$ in view of (21), because they only yield terms proportional to x^{-2}.

Last, the sum $\Sigma^{(c)}$ in (43) has the following asymptotic behavior as $x \to \infty$:

$$\Sigma^{(c)} \sim \left[(3A+9B)x^{-6} + \sum_{k=0}^{\infty}(AC_k + BD_k)x^{-7-k}\right], \tag{50}$$

which yields the following contribution to $\zeta(0)$:

$$\delta_3 = \frac{(3A+9B)}{2} = -3. \tag{51}$$

To sum up, we find

$$\zeta^{Ia}(0) = \delta_1 + \delta_2 + \delta_3 = -\frac{1}{3} - \frac{1}{120} - 3, \tag{52}$$

Therefore, the full $\zeta(0)$ for physical degrees of freedom is given by (cf. (41) and (42))

$$\zeta(0) = \zeta^{Ia}(0) + \frac{5}{2} + \frac{1199}{360} = \frac{112}{45}. \tag{53}$$

3. First Example of Mixed Boundary Conditions on the Whole Set of Metric Perturbations and Ghost Modes

The previous example is very instructive, but of course it would be desirable to compute the effect of boundary conditions on the whole set of metric perturbations and Feynman–DeWitt–Faddeev–Popov ghost fields [25–27]. For this purpose, the work in Ref. [28] studied the following one-parameter family of mixed boundary conditions (with λ being a freely specifiable real parameter):

$$\left[\frac{\partial h_{ij}}{\partial \tau} + \frac{\lambda}{\tau} hij\right]_{\partial M} = 0, \tag{54}$$

$$\left[h_{0i}\right]_{\partial M} = 0, \tag{55}$$

$$\left[h_{00}\right]_{\partial M} = 0, \tag{56}$$

$$\left[\frac{\partial \varphi_i}{\partial \tau} + \frac{\lambda}{\tau} \varphi_i\right]_{\partial M} = 0, \tag{57}$$

$$\left[\frac{\partial \varphi_0}{\partial \tau} + \frac{(\lambda+1)}{\tau} \varphi_0\right]_{\partial M} = 0. \tag{58}$$

With our notation, τ lies in the closed interval $[0, a]$; h_{ij}, h_{0i}, h_{00} are the components of metric perturbations; and φ_i and φ_0 are covariant components of the ghost field of quantum gravity. One therefore deals with transverse-traceless modes, scalar modes, vector modes, decoupled scalar modes, decoupled vector modes, scalar ghost modes, vector ghost modes, and decoupled ghost modes.

A one-parameter family of full $\zeta(0)$ values is therefore obtained [28]:

$$\zeta_\lambda(0) = \frac{89}{90} + \frac{\lambda}{3}(\lambda^2 - 9\lambda - 3). \tag{59}$$

The λ-dependent part of (59) is always positive, either for all

$$\lambda > \frac{9+\sqrt{93}}{2}, \tag{60}$$

or for all

$$\lambda \in \left] \frac{9-\sqrt{93}}{2}, 0 \right[. \tag{61}$$

Equations (60) and (61) are sufficient conditions for the positivity of the full $\zeta_\lambda(0)$, and other suitable values of λ can be computed numerically.

This model is more complete than the one in Section 2, since it deals with all perturbative modes in the one-loop functional integral. However, it still suffers from a non-trivial drawback: the whole set of boundary conditions (54)–(58) is not completely invariant under infinitesimal diffeomorphisms on metric perturbations. For this reason, we resort to the boundary conditions of Section 4.

4. Completely Diff-Invariant Boundary Conditions

The boundary conditions that we study are part of a unified scheme for Maxwell, Yang–Mills, and Quantized General Relativity at one loop, i.e., [29,30]

$$\Big[\pi \mathcal{A}\Big]_{\mathcal{B}} = 0, \tag{62}$$

$$\Big[\Phi(A)\Big]_{\mathcal{B}} = 0, \tag{63}$$

$$[\varphi]_{\mathcal{B}} = 0. \tag{64}$$

With our notation, π is a projector acting on the gauge field $\mathcal{A}$, Φ is the gauge-fixing functional, and φ is the full set of ghost fields. Both Equations (62) and (63) are preserved under infinitesimal gauge transformations provided that the ghost obeys homogeneous Dirichlet conditions as in (64). For gravity, we choose Φ so as to have an operator P of Laplace type on metric perturbations in the one-loop Euclidean theory.

5. Eigenvalue Conditions for Scalar Modes

On the Euclidean four-ball, we expand metric perturbations $h_{\mu\nu}$ in terms of scalar, transverse vector, and transverse-traceless tensor harmonics on S^3. For the vector, tensor, and ghost modes, boundary conditions reduce to Dirichlet or Robin. For scalar modes, one finds eventually the eigenvalues $E = x^2$ from the roots x of [31,32]

$$J_n'(x) \pm \frac{n}{x} J_n(x) = 0, \tag{65}$$

$$J_n'(x) + \left(-\frac{x}{2} \pm \frac{n}{x}\right) J_n(x) = 0. \tag{66}$$

Note that both x and $-x$ solve the same equation.

6. Four Spectral ζ-Functions for Scalar Modes

From Equations (65) and (66), we obtain the following integral representations of the resulting ζ-functions upon exploiting the Cauchy theorem and rotation of contour:

$$\zeta_{A,B}^{\pm}(s) \equiv \frac{(\sin \pi s)}{\pi} \sum_{n=3}^{\infty} n^{-(2s-2)} \int_0^\infty dz\, z^{-2s} \frac{\partial}{\partial z} \log F_{A,B}^{\pm}(zn), \tag{67}$$

where (here $\beta_+ \equiv n, \beta_- \equiv n+2$)

$$F_A^{\pm}(zn) \equiv z^{-\beta_\pm} \Big(zn I_n'(zn) \pm n I_n(zn) \Big), \tag{68}$$

$$F_B^{\pm}(zn) \equiv z^{-\beta_\pm} \left(zn I_n'(zn) + \left(\frac{(zn)^2}{2} \pm n \right) I_n(zn) \right), \tag{69}$$

with I_n being the modified Bessel functions of the first kind. Regularity at the origin is easily proved in the elliptic sectors, corresponding to $\zeta_A^{\pm}(s)$ and $\zeta_B^{-}(s)$.

7. Regularity of ζ_B^+ at $s = 0$

We now define $T \equiv (1+z^2)^{-1/2}$ and consider the uniform asymptotic expansion (away from $T = 1$)

$$z^{\beta_+} F_B^+(zn) \sim \frac{e^{n\eta(T)}}{h(n)\sqrt{T}} \frac{(1-T^2)}{T} \left(1 + \sum_{j=1}^{\infty} \frac{r_{j,+}(T)}{n^j}\right), \tag{70}$$

the functions $r_{j,+}$ being obtained from the Olver polynomials for the uniform asymptotic expansion of I_n and I_n'. On splitting $\int_0^1 dT = \int_0^{\mu} dT + \int_{\mu}^1 dT$ with small μ, we obtain an asymptotic expansion of the l.h.s. by writing, in the first interval on the r.h.s.,

$$\log\left(1 + \sum_{j=1}^{\infty} \frac{r_{j,+}(T)}{n^j}\right) \sim \sum_{j=1}^{\infty} \frac{R_{j,+}(T)}{n^j}, \tag{71}$$

and then computing

$$C_j(\tau) \equiv \frac{\partial R_{j,+}}{\partial T} = (1-T)^{-j-1} \sum_{a=j-1}^{4j} K_a^{(j)} T^a. \tag{72}$$

The integral $\int_{\mu}^1 dT$ is instead found to yield a vanishing contribution in the $\mu \to 1$ limit. Remarkably, by virtue of the spectral identity

$$g(j) \equiv \sum_{a=j}^{4j} \frac{\Gamma(a+1)}{\Gamma(a-j+1)} K_a^{(j)} = 0, \tag{73}$$

which holds $\forall j = 1, \ldots, \infty$, we find

$$\lim_{s \to 0} s\zeta_B^+(s) = \frac{1}{6} \sum_{a=3}^{12} a(a-1)(a-2) K_a^{(3)} = 0, \tag{74}$$

and

$$\zeta_B^+(0) = \frac{5}{4} + \frac{1079}{240} - \frac{1}{2} \sum_{a=2}^{12} \omega(a) K_a^{(3)} + \sum_{j=1}^{\infty} f(j) g(j) = \frac{296}{45}, \tag{75}$$

where

$$\begin{aligned} \omega(a) \quad &\equiv \quad \frac{1}{6} \frac{\Gamma(a+1)}{\Gamma(a-2)} \left[-\log(2) - \frac{(6a^2 - 9a + 1)}{4} \frac{\Gamma(a-2)}{\Gamma(a+1)} \right. \\ &+ \quad \left. 2\psi(a+1) - \psi(a-2) - \psi(4) \right], \end{aligned} \tag{76}$$

$$f(j) \equiv \frac{(-1)^j}{j!} \left[-1 - 2^{2-j} + \zeta_R(j-2)(1 - \delta_{j,3}) + \gamma \delta_{j,3} \right]. \tag{77}$$

The spectral cancellation (73) achieves three goals: (i) vanishing of the $\log 2$ coefficient in Equation (75); (ii) vanishing of $\sum_{j=1}^{\infty} f(j)g(j)$ in Equation (75); and (iii) regularity at the origin of ζ_B^+.

To cross-check our analysis, we evaluate $r_{j,+}(T) - r_{j,-}(T)$ and hence obtain $R_{j,+}(T) - R_{j,-}(T)$ for all j. Only $j = 3$ contributes to $\zeta_B^{\pm}(0)$, and we find

$$\begin{aligned}\zeta_B^{+}(0) &= \zeta_B^{-}(0) - \frac{1}{24}\sum_{l=1}^{4}\frac{\Gamma(l+1)}{\Gamma(l-2)}\left[\psi(l+2) - \frac{1}{(l+1)}\right]\kappa_{2l+1}^{(3)} \\ &= \frac{206}{45} + 2 = \frac{296}{45},\end{aligned} \tag{78}$$

in agreement with Equation (75), where $\kappa_{2l+1}^{(3)}$ are the four coefficients on the right-hand side of

$$\frac{\partial}{\partial T}(R_{3,+} - R_{3,-}) = (1 - T^2)^{-4}\Big(80T^3 - 24T^5 + 32T^7 - 8T^9\Big). \tag{79}$$

Within this framework, the spectral cancellation reads as

$$\sum_{l=1}^{4}\frac{\Gamma(l+1)}{\Gamma(l-2)}\kappa_{2l+1}^{(3)} = 0, \tag{80}$$

which is a particular case of

$$\sum_{a=a_{\min}(j)}^{a=a_{\max}(j)}\frac{\Gamma((a+1)/2)}{\Gamma((a+1)/2 - j)}\kappa_a^{(j)} = 0. \tag{81}$$

Interestingly, the full $\zeta(0)$ value for pure gravity (i.e., including the contribution of tensor, vector, scalar, and ghost modes) is then found to be positive [31,32]:

$$\zeta(0) = \frac{142}{45}, \tag{82}$$

which suggests in light of (5) a quantum avoidance of the cosmological singularity driven by full diffeomorphism invariance of the boundary-value problem for one-loop quantum theory.

8. Open Problems

The DeWitt boundary condition lies at the very heart of deep issues in quantum gravity. As far as we can see, the main open problems are as follows.

(1) Among the three schemes studied in our Sections 2– 7, the latter, i.e., the choice of completely diff-invariant boundary conditions on all perturbative modes, might seem the most satisfactory, but unfortunately, the strong ellipticity of the boundary-value problem is not fulfilled in such a case [30,33–37]. However, our analysis shows that, in the particular case of flat Euclidean four-space bounded by a three-sphere boundary, peculiar cancellations occur, and the resulting $\zeta(0)$ value can be defined and is positive. The deeper underlying reason might be that, in order to define a spectral ζ-function, it is sufficient to find a sector of the complex plane free of eigenvalues of the leading symbol of the elliptic operator under consideration (we are grateful to Professor Gerd Grubb for correspondence about this property a long time ago). An alternative approach might consist in considering non-local boundary conditions in Euclidean quantum gravity [38–40], or the normalizability criterion for the wave function of the universe [41].

(2) The outstanding work in Ref. [10] looked for solutions of the quantum constraint equations in order to check the validity of DeWitt's proposal. However, although one can obtain under suitable assumptions a formal proof of the equivalence of canonical and functional-integral approaches [42], DeWitt himself provided an enlightening example of a sum over histories that does not solve the Wheeler–DeWitt equation [43].

This remark might therefore account for the inequivalence between our conclusions and the results in Ref. [10].

The fascinating question of whether our universe can be non-singular in a semiclassical theory of quantum gravity [44] is therefore still waiting for a fully satisfactory answer.

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Appendix A. The One-Loop Approximation

We are here interested in the approach to quantum field theory in terms of Feynman functional integrals. Hence, we study the amplitudes of going from data on a spacelike surface Σ_1 to data on a spacelike surface Σ_2. For example, in the case of real scalar fields ϕ in a curved background M, the data are the induced three-metric h and a linear combination of ϕ and its normal derivative: $a\phi + b\frac{\partial\phi}{\partial n}$. The latter reduces to homogeneous Dirichlet conditions if $b = 0$, and Neumann conditions if $a = 0$. Otherwise, it is a Robin boundary condition. The quantum amplitudes are functionals of these boundary data. On making a Wick rotation and using the background-field method, we may expand both the four-metric g and the field ϕ about solutions to the classical field equations as $g = g_0 + \overline{g}$ and $\phi = \phi_0 + \overline{\phi}$. However, the more general possibility remains to consider background fields that are not solutions to any field equations, or which are (approximate) solutions in the asymptotic regions. The logarithm of the one-loop functional integral Z for a scalar field (in the main body of our paper, we study pure gravity, but here we focus on scalar fields for simplicity) has an asymptotic expansion

$$\log(Z) \sim \log \int \mu[\overline{\phi}] \mathrm{e}^{-I_2[\overline{\phi}]/\hbar} + \mathrm{O}(\hbar^2), \tag{A1}$$

where μ is a suitable measure of the space of scalar-field perturbations. The part $I_2[\overline{\phi}]$ of the action that is quadratic in scalar-field perturbations involves a second-order elliptic operator $\mathcal{B}$. Assuming completeness of the set $\{\varphi_n\}$ of eigenfunctions of $\mathcal{B}$, with eigenvalues λ_n, the corresponding contribution to one-loop quantum amplitudes involves an infinite product of Gaussian integrals, i.e.,

$$\prod_{n=n_0}^{\infty} \int \mu \, dy_n \, \mathrm{e}^{-\frac{\lambda_n}{2} y_n^2} = \frac{1}{\sqrt{\det\left(\frac{1}{2}\pi^{-1}\mu^{-2}\mathcal{B}\right)}}. \tag{A2}$$

In order to make sense of this infinite product of eigenvalues, one can use ζ-function regularization. This is a rigorous mathematical tool that relies on the spectral theorem, according to which for any elliptic, self-adjoint, and positive-definite operator B, its complex powers B^{-s} can be defined. Hence, its spectral ζ-function is defined as in Equation (4), and the analytic continuation of the ζ-function to the whole complex-s plane takes the form

$$\zeta_B(s) = \sum_{k=-n}^{N} \frac{a_k}{\left(s + \frac{k}{m}\right)} + \phi_N(s), \; k \neq 0. \tag{A3}$$

Thus, on using analytic continuations, $\zeta_B(0)$ is actually finite, and its value gives information about scaling properties of quantum amplitudes. We can now be more precise and describe in detail some key properties. The relation

$$\det B = \mathrm{e}^{-\zeta'(0)} \tag{A4}$$

becomes a possible way to define the determinant of the elliptic operator B upon the analytic continuation of $\zeta_B(s)$. If B is a second-order operator, its eigenvalues λ_n have dimension $(\text{length})^{-2}$. Under conformal rescaling of the metric according to $\widehat{g} = k^2 g$, one has $\widehat{\lambda}_n = \lambda_n / k^2$, and the new spectral ζ-function is $\widehat{\zeta}(s) = k^{2s}\zeta(s)$. This leads to

$$\log\ \det\widehat{B} = \log\ \det B - \log(k^2)\zeta(0), \tag{A5}$$

and hence the partition function scales as

$$\log(\widehat{Z}) = \log(Z) + \frac{1}{2}\log(k^2)\zeta(0) + \log(\widehat{\mu}/\mu)\zeta(0). \tag{A6}$$

The parameter μ is the one occurring in the one-loop semiclassical evaluation of the functional integral. This formula allows for the more general case when the normalization parameter μ changes under scale transformations. One can avoid this complication by assuming that the measure in the functional integral is defined on scalar densities of weight $\frac{1}{2}$.

Equation (A5) can also be used to deduce that the one-loop effective action (for the scalar field) reads as

$$\Gamma^{(1)} = \frac{1}{2}\log\ \det\ \widehat{B} = -\frac{1}{2}\zeta'(0) - \frac{1}{2}\zeta(0)\log(k^2). \tag{A7}$$

Note that the resulting one-loop $\langle \text{out} \mid \text{in} \rangle$ amplitude is measure-dependent unless $\zeta(0) = 0$. This is why $\zeta(0)$ is frequently called the anomalous scaling factor.

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