ESSENTIAL SELF-ADJOINTNESS IN ONE-LOOP QUANTUM COSMOLOGY

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Abstract. The quantization of closed cosmologies makes it necessary to study squared Dirac operators on closed intervals and the corresponding quantum amplitudes. This paper shows that the proof of essential self-adjointness of these second-order elliptic operators is related to Weyl’s limit point criterion, and to the properties of continuous potentials which are positive near zero and are bounded on the interval $[1, \infty[$.

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1. Introduction

One of the fundamental problems of quantum theory is to determine whether the closure of the Hamiltonian operator has self-adjoint extensions [1]. Since each extension leads to a different physics, the problem is not just of technical nature, but lies at the very heart of applied quantum theory [1]. The theory of extensions of symmetric operators is by now a rich branch of modern mathematical physics, and its basic theorems, jointly with many examples, can be found in [1, 2].

On the other hand, in recent years, lots of work have been done on one-loop quantum cosmology and on a rigorous theory of the semiclassical amplitudes when the Dirac operator is considered and local or spectral boundary conditions are imposed [3–7]. Within this framework, the Dirac operator is a first-order elliptic operator which maps primed spinors to unprimed spinors, and the other way around [7, 8]. Using two-component spinor notation [8], the local boundary conditions motivated by local supersymmetry take the form [3, 5–8]

\[ \sqrt{2} \varepsilon n_A A' \psi^A = \pm \psi^{A'} \text{ at } \partial M \]  

(1.1)

where the independent spinor fields \( \left( \psi^A, \bar{\psi}_{A'} \right) \) represent a massless spin-1/2 field, and \( \varepsilon n_A A' \) is the Euclidean normal to the boundary [3, 5]. In [3, 5] it was shown that, on imposing the conditions (1.1) in the case of flat Euclidean backgrounds with boundary, a first-order differential operator exists which is symmetric and has self-adjoint extensions (see also [7, 8]).
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Spectral boundary conditions rely instead on a non-local analysis, i.e. the separation of the spectrum of the intrinsic three-dimensional Dirac operator \( \mathcal{D}_{AB} = e^{n_{AB'}} e^{B'_j} \) \( (3) D_j \) of the boundary into its positive and negative eigenvalues [4, 5]. For example, in the underlying classical theory in the presence of a 3-sphere boundary, the regular modes of the massless field are just the ones which multiply harmonics having positive eigenvalues for \( \mathcal{D}_{AB} \) on \( S^3 \). In the corresponding quantum boundary-value problem, only half of the fermionic field can be freely specified at the boundary (otherwise the problem would be overdetermined), and this is given by the modes which multiply the harmonics on \( S^3 \) having eigenvalues \( \frac{1}{2} (n + \frac{3}{2}) \), with \( n = 0, 1, 2, ... \) [3–5]. With the notation in [4, 5] one thus writes

\[
\psi^A_+ = 0 \quad \text{at} \quad S^3 \tag{1.2}
\]

\[
\tilde{\psi}^{A'}_+ = 0 \quad \text{at} \quad S^3. \tag{1.3}
\]

A naturally occurring question is whether a unique self-adjoint extension for the spin-1/2 boundary-value problem exists, since otherwise different self-adjoint extensions would lead to different spectra and hence the trace anomaly would be ill defined. We shall see that this is not the case, and hence the boundary conditions are enough to determine a unique, real and positive spectrum for the squared Dirac operator (out of which the \( \zeta(0) \) value can be evaluated as in [3–5]).

For this purpose, section 2 presents a brief review of the boundary-value problem for the massless spin-1/2 field. Section 3 proves essential self-adjointness of the squared Dirac operator with spectral boundary conditions, whilst concluding remarks are presented in section 4.
2. The spin-1/2 problem

Following [3–6], we consider flat Euclidean 4-space bounded by a 3-sphere of radius $a$. The spin-1/2 field, represented by a pair of independent (i.e. not related by any conjugation) spinor fields $\psi^A$ and $\tilde{\psi}^{A'}$, is expanded on a family of 3-spheres centred on the origin as [3–6]

$$\psi^A = \frac{1}{2\pi} \tau^{-\frac{3}{2}} \sum_{n=0}^{\infty} \sum_{p,q=1}^{(n+1)(n+2)} \alpha_{n}^{pq} \left[ m_{np}(\tau) \rho^{nqA} + \tilde{r}_{np}(\tau) \sigma^{nqA} \right] \quad (2.1)$$

$$\tilde{\psi}^{A'} = \frac{1}{2\pi} \tau^{-\frac{3}{2}} \sum_{n=0}^{\infty} \sum_{p,q=1}^{(n+1)(n+2)} \alpha_{n}^{pq} \left[ \tilde{m}_{np}(\tau) \rho^{nqA'} + r_{np}(\tau) \sigma^{nqA'} \right]. \quad (2.2)$$

Note that $\tau$ is the Euclidean-time coordinate which plays the role of a radial coordinate, and the block-diagonal matrices $\alpha_{n}^{pq}$ and the $\rho$- and $\sigma$-harmonics are the ones described in detail in [3, 5]. If the boundary conditions (1.1) are imposed, the action functional reduces to a purely volume term [6] and hence takes the form [3, 5, 6]

$$I_E = \frac{i}{2} \int_M \left[ \tilde{\psi}^{A'} \left( \nabla_{AA'} \psi^A \right) - \left( \nabla_{AA'} \tilde{\psi}^{A'} \right) \psi^A \right] \sqrt{\det g} \, d^4x. \quad (2.3)$$

On inserting the expansions (2.1) and (2.2) into the action (2.3), and studying the spin-1/2 eigenvalue equations, one finds that the modes obey the second-order differential equations [3, 5]

$$P_n \tilde{m}_{np} = P_n \tilde{m}_{n,p+1} = P_n \tilde{r}_{np} = P_n \tilde{r}_{n,p+1} = 0 \quad (2.4)$$

$$Q_n r_{np} = Q_n r_{n,p+1} = Q_n m_{np} = Q_n m_{n,p+1} = 0 \quad (2.5)$$
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where \([3, 5]\)

\[ P_n \equiv \frac{d^2}{d\tau^2} + \left[ E_n^2 - \frac{((n+2)^2 - \frac{1}{4})}{\tau^2} \right] \]  
(2.6)

\[ Q_n \equiv \frac{d^2}{d\tau^2} + \left[ E_n^2 - \frac{((n+1)^2 - \frac{1}{4})}{\tau^2} \right] \]  
(2.7)

and \(E_n\) are the eigenvalues of the mode-by-mode form of the Dirac operator \([3, 5]\).

The modes are regular at the origin (\(\tau = 0\)), whilst at the 3-sphere boundary (\(\tau = a\)) they obey the following conditions (which result from (1.1)):

\[-i \ m_{np}(a) = \epsilon \ \tilde{m}_{n,p+1}(a) \]  
(2.8)

\[ i \ m_{n,p+1}(a) = \epsilon \ \tilde{m}_{np}(a) \]  
(2.9)

\[-i \ \tilde{r}_{np}(a) = \epsilon \ r_{n,p+1}(a) \]  
(2.10)

\[ i \ \tilde{r}_{n,p+1}(a) = \epsilon \ r_{np}(a) \]  
(2.11)

where \(\epsilon \equiv \pm 1\).

In the case of spectral boundary conditions, (1.2) and (1.3) imply instead that

\[ m_{np}(a) = 0 \]  
(2.12)

\[ r_{np}(a) = 0. \]  
(2.13)

Thus, one studies the one-dimensional operators \(Q_n\) defined in (2.7), and the eigenmodes are requested to be regular at the origin, and to obey (2.12) and (2.13) on \(S^3\). From now on, we will focus on the spectral case only, since it makes it possible to use the theorems described in the following section.
3. Essential self-adjointness

The previous section shows that we have to study, for all \( n \geq 0 \), the differential operators

\[
\tilde{Q}_n \equiv -\frac{d^2}{d\tau^2} + \frac{((n + 1)^2 - \frac{1}{4})}{\tau^2}.
\]  

(3.1)

These are particular cases of a large class of operators considered in the literature. They can be studied by using the following definitions and theorems from [1, 2]:

**Definition 3.1** The function \( V \) is in the *limit circle* case at zero if for some, and therefore all \( \lambda \), all solutions of the equation

\[
-\varphi''(x) + V(x)\varphi(x) = \lambda \varphi(x) 
\] 

(3.2)

are square integrable at zero.

**Definition 3.2** If \( V(x) \) is not in the limit circle case at zero, it is said to be in the *limit point* case at zero.

**Theorem 3.1** (Weyl’s limit point - limit circle criterion) Let \( V \) be a continuous real-valued function on \((0, \infty)\). Then \( \mathcal{O} \equiv -\frac{d^2}{dx^2} + V(x) \) is essentially self-adjoint on \( C_0^\infty(0, \infty) \) if and only if \( V(x) \) is in the limit point case at both zero and infinity.

**Theorem 3.2** Let \( V \) be continuous and positive near zero. If \( V(x) \geq \frac{3}{4}x^{-2} \) near zero, then \( \mathcal{O} \) is in the limit point case at zero.

**Theorem 3.3** Let \( V \) be differentiable on \( ]0, \infty[ \) and bounded above by \( K \) on \([1, \infty[ \). Suppose that


(i) \[ \int_1^\infty \frac{dx}{\sqrt{K-V(x)}} = \infty. \]

(ii) \[ V'(x)|V(x)|^{-\frac{3}{2}} \text{ is bounded near infinity.} \]

Then \( V(x) \) is in the limit point case at \( \infty \).

In other words, a necessary and sufficient condition for the existence of a unique self-adjoint extension, is that the eigenfunctions of \( \mathcal{O} \) should fail to be square integrable at zero and at infinity. We will not give many technical details, since we are more interested in the applications of the general theory. However, we find it helpful for the general reader to point out that, when \( V(x) \) takes the form \( \frac{c}{x^2} \) for \( c > 0 \), theorem 3.2 can be proved as follows [1]. The equation

\[ -\varphi''(x) + \frac{c}{x^2} \varphi(x) = 0 \quad (3.3) \]

admits solutions of the form \( x^\alpha \), where \( \alpha \) takes the values

\[ \alpha_1 = \frac{1}{2} + \frac{1}{2} \sqrt{1 + 4c} \quad (3.4) \]

\[ \alpha_2 = \frac{1}{2} - \frac{1}{2} \sqrt{1 + 4c}. \quad (3.5) \]

When \( \alpha = \alpha_1 \) the solution is obviously square integrable at zero. However, when \( \alpha = \alpha_2 \), the solution is square integrable at zero if and only if \( \alpha_2 > -\frac{1}{2} \), which implies \( c < \frac{3}{4} \). By virtue of definitions 3.1 and 3.2, this means that \( V(x) \) is in the limit point at zero if and only if \( c \geq \frac{3}{4} \).

However, in our problem we are interested in the closed interval \([0,a]\), where \( a \) is finite. Thus, the previous theorems can only be used after relating the original problem to another one involving the infinite interval \((0,\infty)\). For this purpose, we perform a double
change of variables. The first one affects the independent variable, whereas the second one is performed on the dependent variable so that the operator takes the form (3.2) with the appropriate (semi)infinite domain.

Given (3.3) with \( x \in [0, a] \) (see (3.1)) we perform the change

\[
x \equiv a \left(1 - e^{-y}\right) \Rightarrow y \in (0, \infty).
\]

This yields the equation

\[
\ddot{\varphi}(y) + \dot{\varphi}(y) - \frac{c(n)}{(e^y - 1)^2} \varphi(y) = 0 \quad y \in (0, \infty)
\]

where \( c(n) \equiv (n+1)^2 - \frac{1}{4} \) and the dot denotes differentiation with respect to \( y \). The further change

\[
\varphi(y) \equiv e^{-\frac{y}{2}} \chi(y)
\]

leads to

\[
-\ddot{\chi}(y) + \left[ \frac{1}{4} + \frac{c(n)}{(e^y - 1)^2} \right] \chi = 0 \quad y \in (0, \infty)
\]

which has the structure of the left hand side of (3.2) with a suitable domain, so that Weyl’s theorem is directly applicable. Indeed, when \( y \to \infty \), the conditions (i) and (ii) of theorem 3.3 are clearly satisfied by the potential in (3.9), and hence such a \( V(y) \) is in the limit point at \( \infty \) (in that case, the constant of theorem 3.3 is \( K(n) \equiv \frac{1}{4} + \frac{c(n)}{(e-1)^2} \)). Moreover, when \( y \to 0 \), \( V(y) \) tends to \( \frac{1}{4} + \frac{c(n)}{y^2} \geq \frac{1}{4} + \frac{3}{4} \frac{1}{y^2} \), since \( n \geq 0 \) in (3.1). Thus, the condition of theorem 3.2 is satisfied and we are in the limit point at zero as well. By virtue of theorem
3.1, these properties imply that our operators (3.1) are related, through (3.6) and (3.8), to the second-order elliptic operators

\[ T_n \equiv -\frac{d^2}{dy^2} + \frac{1}{4} + \frac{(n + 1)^2 - \frac{1}{4}}{(e^y - 1)^2} \]  

(3.10)

which are essentially self-adjoint on the space of \( C^\infty \) functions on \((0, \infty)\) with compact support (see section 4).

4. Concluding remarks

There is indeed a rich mathematical literature on self-adjointness properties of the Dirac operator (see, for example, [9] and references therein). However, one-loop quantum cosmology needs a rigorous proof of essential self-adjointness of elliptic operators with local or non-local boundary conditions. Our paper represents the first step in this direction, in the case of the squared Dirac operator with the spectral boundary conditions (1.2) and (1.3) [4, 5]. Note that such non-local boundary conditions play a crucial role in section 3.

As shown on page 153 of [1], to prove theorem 3.1 one has to choose at some stage a point \( c \in (0, \infty) \) and then consider the operator

\[ A \equiv -\frac{d^2}{dx^2} + V(x) \]

on the domain

\[ D(A) \equiv \{ \omega : \omega \in C^\infty(0, c), \omega = 0 \text{ near zero}, \omega(c) = 0 \} . \]
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As far as we can see, this scheme is only compatible with the boundary conditions (2.12) and (2.13), which result from the spectral choice (1.2) and (1.3). Thus, we should stress that the extension to the boundary conditions (2.8)–(2.11) resulting from (1.1) remains the main open problem in our investigation.

In this respect, we should also emphasize that, in the differential equations viewpoint, one focuses on the boundary conditions, whilst in the functional analysis viewpoint the key elements are the domains of differential operators. Strictly, the domain corresponding to a given choice of boundary conditions may also contain some less well behaved functions (we thank Bernard Kay for clarifying this point).

Moreover, it remains to be seen how to apply similar techniques to the analysis of higher-spin fields. These are gauge fields and gravitation, which obey a complicated set of mixed boundary conditions [10–13]. If this investigation could be completed, it would put on solid ground the current work on trace anomalies and one-loop divergences on manifolds with boundary [3–5, 10–13], and it would add evidence in favour of quantum cosmology being at the very heart of many exciting developments in quantum field theory, analysis and differential geometry [3–5, 12, 13].

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In our paper we study the differential operator

\[ \tilde{Q}_n \equiv -\frac{d^2}{d\tau^2} + \frac{((n+1)^2 - \frac{1}{4})}{\tau^2} \]

where \( \tau \in [0, a] \) and \( n = 0, 1, 2, \ldots \), with domain given by the functions \( u \) in \( AC^2[0, a] \) such that \( u(a) = 0 \). The operator \( \tilde{Q}_n \) obeys the limit point condition at \( \tau = 0 \), as we prove in the paper, and the limit circle condition at \( \tau = a \). These properties, jointly with the homogeneous Dirichlet condition at \( \tau = a \), are sufficient to obtain a self-adjoint boundary-value problem. Thus, there is no need to change independent and dependent variable as we did. Moreover, our changes of variable lead actually to the operator

\[ \tilde{T}_n \equiv a^{-2}e^{2y} \left[ -\frac{d^2}{dy^2} + \frac{1}{4} + \frac{(n+1)^2 - \frac{1}{4}}{(e^y - 1)^2} \right] \]

where \( y \) ranges from 0 through \( \infty \). The Weyl limit point-limit circle criterion stated in our Theorem 3.1 ensures that the operator \( O \equiv -\frac{d^2}{dx^2} + V(x) \) is essentially self-adjoint on \( C_0^\infty(0, \infty) \) if and only if \( V(x) \) is in the limit point at both zero and infinity. To check this, it is indeed sufficient to study the eigenvalue equation \( O\varphi(x) = \lambda\varphi(x) \) for a particular value of \( \lambda \), e.g. \( \lambda = 0 \). We had instead considered the zero-eigenvalue equation in the transformed variables leading to \( \tilde{T}_n \), because \( \tilde{Q}_n \) is not studied on \( (0, \infty) \). But this was not enough, because the corresponding scalar product is no longer

\[ (u, v) \equiv \int_0^1 u^*(\tau)v(\tau) d\tau \]
but

$$\langle u, v \rangle \equiv \int_0^\infty u^*(y)v(y)e^{-2y}dy$$

and the counterpart (if any) of the Weyl criterion for the operator $\tilde{T}_n$ remains to be elaborated.

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