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by

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Abstract

The spectral problem where the field satisfies Dirichlet conditions on one part of the boundary of the relevant domain and Neumann on the remainder is discussed. It is shown that there does not exist a classical asymptotic expansion for short time in terms of fractional powers of t with locally computable coefficients. MSC Classification: 58G25

1 Introduction

Let M be a compact m dimensional Riemannian manifold with smooth boundary ∂M. Let D be an operator of Laplace type on the space of smooth sections to a vector bundle V. Let $D_{\mathcal{B}}$ be the realization of D with respect to the boundary conditions defined by a suitable local boundary operator $\mathcal{B}$; we assume $D_{\mathcal{B}}$ is self adjoint. In this paper, we shall study the heat trace asymptotics.

We begin by reviewing the situation in the classical setting and refer to [14, 16, 30] for further details. We suppose given a decomposition of $\partial M = C_N \cup C_D$ as the *disjoint* union of two closed (possibly empty) sets. On ∂M, let $u_{;m}$ be the covariant derivative of u with respect to the inward unit normal; we use the natural connection defined by D – see [10] for details. Let the boundary operator

$$\mathcal{B}u := u|_{C_D} \oplus (u_{;m} + Su)|_{C_N}$$

define Dirichlet boundary conditions on C_D and Robin boundary conditions on C_N. Let ϕ be the initial temperature distribution. The subsequent heat

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temperature distribution $u := e^{-tD_{\mathcal{B}}}\phi$ is defined by the equations:

$$(\partial_t + D)u = 0,\ u(0;x) = \phi(x),\ \text{and } \mathcal{B}u = 0.$$

Let $\{\phi_i, \lambda_i\}$ be a discrete spectral resolution of $D_{\mathcal{B}}$; the ϕ_i are smooth sections of V which form a complete orthonormal basis for $L^2(V)$ so that

$$\mathcal{B}\phi_i = 0 \text{ and } D\phi_i = \lambda_i\phi_i.$$

The fundamental solution of the heat equation is trace class. We define

$$a(D,\mathcal{B})(t) := \mathrm{Tr}_{L^2} e^{-tD_{\mathcal{B}}} = \textstyle\sum_i e^{-t\lambda_i}.$$

Theorem 1 *Let $C_N \cap C_D = \emptyset$. The heat trace $a(D,\mathcal{B})(t)$ has a complete asymptotic expansion as $t \downarrow 0$ of the form:*

$$a(D,\mathcal{B})(t) \sim \textstyle\sum_{n\geq 0} a_n(D,\mathcal{B}) t^{(n-m)/2}.$$

The asymptotic coefficients are locally computable as the integral of smooth local invariants:

$$\begin{aligned} a_n(D,\mathcal{B}) &= \textstyle\int_M a_n(x,D)dx + \int_{C_N} a_n^+(y,D,\mathcal{B})dy \\ &\quad + \textstyle\int_{C_D} a_n^-(y,D,\mathcal{B})dy. \end{aligned}$$

These invariants have been computed for $n \leq 5$, see for example [4, 5, 19, 23, 24]. There exists a canonical connection ∇ and a canonical endomorphism E so that $D = -\mathrm{Tr}(\nabla^2 + E)$. If D is the Laplacian on p forms, then ∇ is the Levi-Civita connection and E is given in terms of the Riemann curvature tensor R by the Weitzenböck formulas. Let indices i, j range from 1 through m and index a local orthonormal frame $\{e_i\}$ for the tangent bundle of M. Near the boundary we choose an orthonormal frame so e_m is the inward unit normal; let indices a, b range from 1 through $m-1$ and index the induced frame for the tangent bundle of the boundary. Let $L_{ab}^{\partial M}$ be the second fundamental form of $\partial M \subset M$. We adopt the Einstein convention and sum over repeated indices.

Theorem 2

1. $a_0(D,\mathcal{B}) = (4\pi)^{-m/2} \int_M \mathrm{Tr}\,(I_V)$.
2. $a_1(D,\mathcal{B}) = (4\pi)^{(1-m)/2} \frac{1}{4} \{ \int_{C_N} \mathrm{Tr}\,(I_V) - \int_{C_D} \mathrm{Tr}\,(I_V) \}$.

3. $a_2(D,\mathcal{B}) = (4\pi)^{-m/2}\frac{1}{6}\{\int_M \operatorname{Tr}(R_{ijji}I_V + 6E) + \int_{C_N} \operatorname{Tr}(2L_{aa}I_V + 12S)$
$+ \int_{C_D} \operatorname{Tr}(2L_{aa}I_V)\}$.

4. $a_3(D,\mathcal{B}) = -(4\pi)^{(1-m)/2}\frac{1}{384}\{\int_{C_N} \operatorname{Tr}(96E + 96SL_{aa} + 192S^2$
$+(16R_{ijji} - 8R_{amma} + 13L_{aa}L_{bb} + 2L_{ab}L_{ab})I_V)$
$+ \int_{C_D} \operatorname{Tr}(96E + (16R_{ijji} - 8R_{amma} + 7L_{aa}L_{bb} - 10L_{ab}L_{ab})I_V)\}$.

In the classical setting, $C_N \cap C_D$ is empty so the Neumann and Dirichlet components do not overlap. There are, however, physically reasonable settings where $\Sigma := C_D \cap C_N$ is a non–empty smooth submanifold of ∂M of dimension $m-2$. Drop a solid ball at initial temperature ϕ into icewater. Supposing it floats, the part of the boundary of the ball which is in air satisfies Neumann conditions and the part underwater satisfies Dirichlet conditions. Here, $\mathcal{B}$ is defined by complementary spherical caps about the north and south poles of the ball which intersect in a circle of latitude.

The setting where Σ is not empty is known in the literature as the N/D problem. It has been investigated extensively from the functional analytic point of view [20, 25, 26, 29]. However, there are only some preliminary results [2, 3, 6] available concerning the heat trace asymptotics. It is natural to conjecture that Theorem 1 can be generalized to this setting by adding an extra integral over Σ of some suitably chosen local invariant. The point of this note is to indicate that the situation is not quite so simple. More specifically, we will show that the following conjecture is **false**.

Conjecture 3 *Let $C_N \cap C_D$ be a smooth hypersurface in ∂M. The heat trace $a(D,\mathcal{B})(t)$ has a complete asymptotic expansion as $t \downarrow 0$ of the form:*

$$a(D,\mathcal{B})(t) \sim \textstyle\sum_{n\geq 0} a_n(D,\mathcal{B})t^{(n-m)/2}.$$

The asymptotic coefficients are locally computable as the integral of smooth local invariants:

$$\begin{aligned} a_n(D,\mathcal{B}) &= \textstyle\int_M a_n(x,D)dx + \int_{C_N} a_n^+(y,D,\mathcal{B})dy \\ &\quad + \textstyle\int_{C_D} a_n^-(y,D,\mathcal{B})dy + \int_\Sigma a_n^\Sigma(z,D,\mathcal{B})dz. \end{aligned}$$

Here is a brief outline to the paper. We shall suppose that Conjecture 3 holds and argue for a contradiction. In §2, we discuss some of the functorial properties which the invariants a_n^Σ would have. In §3, we use the local index formula in a specific situation to show Conjecture 3 is false at the a_3 level. In §4 we present some results using a perturbation expansion around an exactly soluble, but restricted, case which also relate to this question. In §5 we conclude by suggesting an alternative form that the expansion might take.

2 Properties of the local invariants

We use dimensional analysis to study these invariants; this involves studying the behavior of the heat trace under rescaling. Let Ω be the curvature tensor of the connection determined by D. We assign weight 2 to the tensors R, Ω, and E. We assign weight 1 to the tensors S and L. We increase the weight by 1 for each explicit covariant derivative which appears. It then follows that the integrands which can be used to compute the invariants $(a_n^M, a_n^\pm, a_n^\Sigma)$ are universal polynomials which are weighted homogeneous of degrees $(n, n-1, n-2)$. For example, Theorem 2 expresses a_2 in terms of an interior integral of $\mathrm{Tr}\,(R_{ijji}I_V + 6E)$ and boundary integrals of $\mathrm{Tr}\,(2L_{aa})$ and $\mathrm{Tr}\,(2L_{aa} + 12S)$; these expressions have weights $(2, 1, 1)$. Thus we see that

$$a_0^\Sigma = 0,\ a_1^\Sigma = 0,\ \text{and}\ a_2^\Sigma = c_0 \dim(V).$$

Calculations of Avramidi [2, 3] and of Dowker [6] suggest that

$$c_0 = -\tfrac{\pi}{4}(4\pi)^{-m/2}.$$

We shall work with the a_3^Σ coefficient to show Conjecture 3 fails. Let L^Σ be the second fundamental form of $\Sigma \subset C_N$. Any invariant which is homogeneous of weight 1 can be expressed linearly in terms of the tensors $\{S, L^\Sigma, L^{\partial M}\}$. Thus, in particular, the geometry of the operator D does not enter into a_3^Σ. We choose a local frame field on Σ so that e_{m-1} is the unit normal of $\Sigma \subset C_N$ and so that e_m is the unit normal of $C_N \subset M$. Thus the structure group is $O(m-2)$. Let $1 \le u \le m-2$. We use H. Weyl's theorem [31] on the invariants of the orthogonal group to see there exist universal constants c_i so that

$$a_3^\Sigma(z, D, \mathcal{B}) = \mathrm{Tr}\,\{(c_1 L_{uu}^\Sigma + c_2 L_{uu}^{\partial M} + c_3 L_{m-1,m-1}^{\partial M})I_V + c_4 S\}. \qquad (1)$$

Let $M = M_1 \times M_2$ where M_2 is a closed manifold. Let $D := D_1 \otimes 1 + 1 \otimes D_2$ where the operators D_i are operators of Laplace type over M_i. We use a suitable boundary condition $\mathcal{B}_1$ for D_1 to induce a corresponding boundary condition $\mathcal{B}$ for D. The discrete spectral resolution for $(D, \mathcal{B})$ is given by the tensor product of the corresponding discrete spectral resolutions for $(D_1, \mathcal{B}_1)$ and D_2. Therefore

$$\begin{aligned}
&a(D,\mathcal{B})(t) = a(D_1,\mathcal{B}_1)(t)\cdot a(D_2)(t) \text{ so} \\
&a_n(x,D) = \textstyle\sum_{p+q=n} a_p(x_1,D_1)a_q(x_2,D_2), \\
&a_n^{\pm}(y,D,\mathcal{B}) = \textstyle\sum_{p+q=n} a_p^{\pm}(y_1,D_1,\mathcal{B}_1)a_q(x_2,D_2), \text{ and} \\
&a_n^{\Sigma}(z,D,\mathcal{B}) = \textstyle\sum_{p+q=n} a_p^{\Sigma}(z_1,D_1,\mathcal{B}_1)a_q(x_2,D_2).
\end{aligned} \tag{2}$$

A priori, the constants c_i of equation (1) could depend on the dimension m but the usual trick of dimension shifting using equation (2) and taking product with a circle shows the constants c_i are dimension free modulo a multiplicative normalizing factor involving suitable powers of 4π.

We say that an operator $A : C^\infty(V_1) \to C^\infty(V_2)$ is of *Dirac type* if the associated second order operators $D^1 := A^*A$ and $D^2 := AA^*$ are of Laplace type. We assume given boundary conditions $\mathcal{B}^i$ so that A intertwines the spectral resolutions of $D^1_{\mathcal{B}^1}$ and $D^2_{\mathcal{B}^2}$. We define:

$$\text{index}(A) := \dim\ \ker(D^1_{\mathcal{B}^1}) - \dim\ \ker(D^2_{\mathcal{B}^2}).$$

The cancellation argument of Bott then shows

$$\begin{aligned}
&a_m(D^1,\mathcal{B}^1) - a_m(D^2,\mathcal{B}^2) = \text{index}(A) \text{ and} \\
&a_n(D^1,\mathcal{B}^1) - a_n(D^2,\mathcal{B}^2) = 0 \text{ if } n \neq m.
\end{aligned} \tag{3}$$

We shall apply this observation in §3 to the de Rham complex with absolute or relative boundary conditions. McKean and Singer [21] used equation (3) to prove the Gauss-Bonnet theorem if $m = 2$; we refer to [11] for a discussion of the higher dimensional setting.

3 An example on the cylinder

Let $M := [0,1] \times S^2$ be the cylinder with the standard product metric. We consider the de Rham complex and let $\Lambda^{e,o}$ be the bundle of even and odd differential forms. Let $D^{e,o}$ be the associated Laplacians. Let $x \in [0,1]$ be the normal variable and let $\Theta \in S^2$ be the angular variable. We then have natural decompositions:

$$\begin{aligned}
&\Lambda^e_M = \Lambda^e_S \oplus dx \wedge \Lambda^o_S,\ D^e_M = (-\partial_x^2 + \Delta^e_S) \oplus (-\partial_x^2 + \Delta^o_S) \\
&\Lambda^o_M = \Lambda^o_S \oplus dx \wedge \Lambda^e_S,\ D^o_M = (-\partial_x^2 + \Delta^o_S) \oplus (-\partial_x^2 + \Delta^e_S).
\end{aligned} \tag{4}$$

If $\phi_i \in C^\infty(\Lambda_S)$ are differential forms on M taking values in Λ_S, then absolute and relative boundary conditions are defined by the operators:

$$\begin{aligned}\mathcal{B}_a(\phi_1 + dx \wedge \phi_2) &:= \{\partial_x(\phi_1) \oplus \phi_2\} \text{ and}\\ \mathcal{B}_r(\phi_1 + dx \wedge \phi_2) &:= \{\partial_x(\phi_2) \oplus \phi_1\}.\end{aligned}$$

We have

$$\begin{aligned}&(d+\delta)_M(\phi_1 + dx \wedge \phi_2)\\ &\quad = \{-\partial_x\phi_2 + (d+\delta)_S\phi_1\} + dx \wedge \{\partial_x\phi_1 - (d+\delta)_S\phi_2\}.\end{aligned}$$

Suppose that $\Delta\phi = \lambda\phi$ on M. If $\mathcal{B}^a\phi = 0$ on an open subset $\mathcal{O} \subset \partial M$, then

$$\begin{aligned}&\partial_x\{-\partial_x\phi_2 + (d+\delta)_S\phi_1\}|_{\mathcal{O}}\\ &\quad = (-\Delta_S + \lambda)\{\phi_2|_{\mathcal{O}}\} + (d+\delta)_S\{\partial_x\phi_1|_{\mathcal{O}}\} = 0 \text{ and}\\ &\{\partial_x\phi_1 - (d+\delta)_S\phi_2\}|_{\mathcal{O}} = -(d+\delta_S)\{\phi_2|_{\mathcal{O}}\} = 0\end{aligned}$$

so $\mathcal{B}^a\{(d+\delta)\phi\} = 0$ on $\mathcal{O}$. Similarly if $\mathcal{B}^r\phi = 0$ on $\mathcal{O}$, then

$$\begin{aligned}&\{-\partial_x\phi_2 + (d+\delta)_S\phi_1\}|_{\mathcal{O}} = (d+\delta_S)\{\phi_1|_{\mathcal{O}}\} = 0 \text{ and}\\ &\partial_x\{\partial_x\phi_1 - (d+\delta)_S\phi_2\}|_{\mathcal{O}}\\ &\quad = (\Delta_S - \lambda)\{\phi_1|_{\mathcal{O}}\} - (d+\delta)_S\{\partial_x\phi_2|_{\mathcal{O}}\} = 0\end{aligned}$$

so $\mathcal{B}^r\{(d+\delta)\phi\} = 0$ on $\mathcal{O}$. Thus $(d+\delta)$ preserves the eigenforms of the Laplacian with either absolute or relative boundary conditions.

Let $\mathcal{B}^-$ denote pure Dirichlet and $\mathcal{B}^+$ pure Neumann boundary conditions. The structures decouple and we may decompose

$$\begin{aligned}(D_M^e, \mathcal{B}_a) &= (-\partial_x^2 + \Delta_S^e, \mathcal{B}^+) \oplus (-\partial_x^2 + \Delta_S^o, \mathcal{B}^-)\\ (D_M^o, \mathcal{B}_a) &= (-\partial_x^2 + \Delta_S^e, \mathcal{B}^-) \oplus (-\partial_x^2 + \Delta_S^o, \mathcal{B}^+)\\ (D_M^e, \mathcal{B}_r) &= (-\partial_x^2 + \Delta_S^e, \mathcal{B}^-) \oplus (-\partial_x^2 + \Delta_S^o, \mathcal{B}^+)\\ (D_M^o, \mathcal{B}_r) &= (-\partial_x^2 + \Delta_S^e, \mathcal{B}^+) \oplus (-\partial_x^2 + \Delta_S^o, \mathcal{B}^-).\end{aligned}$$

The interior invariants vanish if n is odd. Thus for dimensional reasons,

$$a_3(D_M^e)(x,\Theta) = 0 \text{ and } a_3(D_M^o)(x,\Theta) = 0. \tag{5}$$

We use Theorem 2 (2) to see that

$$a_1^\pm(y, -\partial_x^2, \mathcal{B}^\pm) = \pm\tfrac{1}{4} \text{ for } y \in \partial[0,1].$$

The Dirichlet and Neumann boundary conditions for Δ decouple on S^2. Since the structures on M are product, we may apply equation (2) with $n = 3$, $p = 1$, and $q = 2$ to the decompositions of display (4) to compute:

$$\begin{aligned}
a_3^{\partial M}(D_M^e, \mathcal{B}_a)(y,\Theta) &= \tfrac14\{a_2^S(\Theta,\Delta_S^e) - a_2^S(\Theta,\Delta_S^o)\},\\
a_3^{\partial M}(D_M^o, \mathcal{B}_a)(y,\Theta) &= \tfrac14\{-a_2^S(\Theta,\Delta_S^e) + a_2^S(\Theta,\Delta_S^o)\},\\
a_3^{\partial M}(D_M^e, \mathcal{B}_r)(y,\Theta) &= \tfrac14\{-a_2^S(\Theta,\Delta_S^e) + a_2^S(\Theta,\Delta_S^o)\},\\
a_3^{\partial M}(D_M^o, \mathcal{B}_r)(y,\Theta) &= \tfrac14\{a_2^S(\Theta,\Delta_S^e) - a_2^S(\Theta,\Delta_S^o)\}
\end{aligned}$$

for $y \in \partial\{[0,1]\}$. McKean and Singer [21] showed that

$$a_2^S(\Theta,\Delta_S^e) - a_2^S(\Theta,\Delta_S^o) = \tfrac{1}{2\pi};$$

this also follows from Theorem 2 since $E = 0$ for Δ_S^e while $\mathrm{Tr}\,E = -2R_{ijji}$ for Δ_S^o. Consequently, we compute the index densities:

$$\begin{aligned}
\{a_3^{\partial M}(D_M^e,\mathcal{B}_a) - a_3^{\partial M}(D_M^o,\mathcal{B}_a)\}(y,\Theta) &= \tfrac{1}{4\pi}\\
\{a_3^{\partial M}(D_M^e,\mathcal{B}_r) - a_3^{\partial M}(D_M^o,\mathcal{B}_r)\}(y,\Theta) &= -\tfrac{1}{4\pi}
\end{aligned} \tag{6}$$

Let $C_{a,S} \subset S^2$ and $C_{r,S} \subset S^2$ be complementary spherical caps about the north and south pole in S^2. Let $C_{a,M} := \{0,1\}\times C_{a,S}$ and $C_{r,M} := \{0,1\}\times C_{r,S}$ give a corresponding decomposition of the boundary of M. Let $\mathcal{B}$ be the boundary condition $\mathcal{B}_a$ on $C_{a,M}$ and $\mathcal{B}_r$ on $C_{r,M}$. The decompositions of display (4) induces corresponding decompositions of $\mathcal{B}$ as the sum of two boundary conditions of the form we have been considering:

$$\begin{aligned}
\mathcal{B}(\phi_i) &= \phi_i|_{C_{a,M}} \oplus (\partial_x\phi_i)|_{C_{r,M}} \text{ and}\\
\mathcal{B}(dx\wedge\phi_i) &= (\partial_x\phi_i)|_{C_{a,M}} \oplus \phi_i|_{C_{r,M}}
\end{aligned}$$

As the metric is product, $L_{aa}^{\partial M} = 0$. Since $S = 0$, the only non-zero term in a_3^Σ given in equation (1) is $c_1 L_{uu}^\Sigma \mathrm{Tr}\,(I)$. This term is sensitive to the normal of $\Sigma \subset \partial M$. When studying D_M^e or D_M^o we have D/N boundary conditions on half the bundle and N/D boundary conditions on the other half the bundle. Thus this term cancels and we have

$$a_3^\Sigma(D_M^e,\mathcal{B})(x,\Theta) = 0 \text{ and } a_3^\Sigma(D_M^o,\mathcal{B})(x,\Theta) = 0. \tag{7}$$

We may therefore use equation (5), equation (6), and equation (7) to see

$$a_3(D_M^e,\mathcal{B}) - a_3(D_M^o,\mathcal{B}) = \tfrac{1}{2\pi}\{\mathrm{vol}(C_{a,M}) - \mathrm{vol}(C_{r,M})\}.$$

Thus this difference is not an integer if the spherical caps are not hemispheres. On the other hand, since $d+\delta$ intertwines the eigenvalues of the Laplacian with either absolute or relative boundary conditions, we can use equation (3) to see that

$$a_3(D_M^e,\mathcal{B}) - a_3(D_M^o,\mathcal{B}) = \mathrm{index}(d+\delta,\mathcal{B}) \in \mathbb{Z}.$$

This contradiction shows that Conjecture 3 is false.

4 Special cases and perturbative expansions

The special case of the N/D wedge has been considered locally by Avramidi [3] and globally by Dowker [6], where the N/D hemisphere problem was also introduced. In this section we first enlarge on this last example for which the N/D problem can be solved explicitly in terms of known functions, and then perturb it to give a more general geometry.

Consider the hemisphere placed at $y \geq 0$ such that its boundary is at $\varphi = 0$ and $\varphi = \pi$ with $\theta \in [0,\pi]$. The metric in the standard (θ,φ) polar coordinates and the Laplacian are given by:

$$ds^2 = d\theta^2 + \sin^2\theta d\varphi^2 \text{ and } \Delta = -\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} - \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}.$$

We are interested in the eigenfunctions $Y(\varphi,\theta)$ which satisfy the N/D boundary condition. To get an idea of the crucial difference between these conditions and the classical Dirichlet and Neumann ones, we will provide details for all of them.

The starting point is the separation of variables, $Y(\varphi,\theta) = \Phi(\varphi)\Xi(\theta)$, which leads to the usual differential equations:

$$\begin{aligned} 0 &= \Phi''(\varphi) + \mu^2\Phi(\varphi) \\ 0 &= \sin\theta(\sin\theta\ \Xi'(\theta))' + (\lambda^2\sin^2\theta - \mu^2)\Xi(\theta). \end{aligned}$$

With the substitution $\xi = \cos\theta$, $\Xi(\theta) = u(\xi)$, one finds

$$0 = (1-\xi^2)u''(\xi) - 2\xi u'(\xi) + \left(\lambda^2 - \frac{\mu^2}{1-\xi^2}\right)u(\xi).$$

The general solution for Φ is $\Phi(\varphi) = a\sin(\mu\varphi) + b\cos(\mu\varphi)$, with $a,b \in \mathbb{C}$. The equation for u is the differential equation of the associated Legendre functions. Which eigenfunctions survive as being linearly independent depends on the value of μ and thus on the boundary condition. We refer to [27] for further details.

4.1 Dirichlet boundary conditions mean that $\Phi(0) = \Phi(\pi) = 0$ and hence $\mu \in \mathbb{N}$. Independent solutions are $P_l^\mu(\xi)$ and $Q_l^\mu(\xi)$ with $l \geq \mu$, $l \in \mathbb{N}$, and eigenvalues $\lambda^2 = l(l+1)$. Imposing square integrability on the eigenfunctions shows that the discrete spectral resolution is given by the functions:

$$Y(\varphi, \theta) = \mathcal{N}_1 \sin(\mu\varphi) P_l^\mu(\cos\theta), \quad \mu \in \mathbb{N}, \quad l = n + \mu, \quad n \in \mathbb{N}_0, \tag{8}$$

with $\mathcal{N}_1$ a normalization constant. For $\theta \to 0$ and $\theta \to \pi$, which is the limit to the north and south poles, we see that

$$P_l^\mu(\cos\theta) \sim (1 - \cos^2\theta)^{\mu/2} = (\sin\theta)^\mu$$

and so the eigenfunctions are differentiable at the poles, which of course, must be the case. We refer to [15] for further details.

4.2 Neumann boundary conditions mean that $\Phi'(0) = \Phi'(\pi) = 0$. This yields the quantization condition, $\mu \in \mathbb{N}_0$ and, arguing as before, we see that the discrete spectral resolution is given by the functions:

$$Y(\varphi, \theta) = \mathcal{N}_2 \cos(\mu\varphi) P_l^\mu(\cos\theta), \quad \mu \in \mathbb{N}_0, \quad l = n + \mu, \quad n \in \mathbb{N}_0.$$

Again, these are differentiable everywhere, including the poles.

4.3 N/D boundary conditions mean that $\Phi(0) = \Phi'(\pi) = 0$. Consequently $\mu = n + 1/2$, $n \in \mathbb{N}_0$, or, stated differently, $\mu = \bar{m}/2$, $\bar{m} = 1, 3, 5, ...$ Thus the discrete spectral resolution is given by the functions:

$$Y(\varphi, \theta) = \mathcal{N}_3 \sin(\mu\varphi) P_l^{-\mu}(\cos\theta), \quad \mu = \tfrac{\bar{m}}{2}, \quad \bar{m} = 1, 3, 5, ..., \quad n \in \mathbb{N}_0\,,$$

with $l = n + \mu$. The vital difference is that now μ is a half-integer for which the limiting behaviour of the eigenfunctions near the poles, *i.e.* the edge, is

$$P_l^{-\bar{m}/2}(\cos\theta) \sim (\sin\theta)^{\bar{m}/2},$$

so that the eigenfunctions are not differentiable at the edge. This is the crucial difference between the N/D problem and the classical problems, and is responsible for the non-standard small-t behaviour of the heat-trace.

Having given the eigenfunctions for the hemisphere, for which the boundary extrinsic curvature vanishes, we now provide a perturbation approach which allows account to be taken of the influence of an extrinsic curvature at a boundary. Some general developments are given first and applied to the hemisphere later.

Assume the unperturbed situation $\Delta\phi_\lambda = \lambda^2\phi_\lambda$ with $\phi|_{\partial\mathcal{M}} = 0$ with non-degenerate eigenvalues. Parametrise the boundary by y and take $s(y)$ to be the geodesic distance from it. We define the perturbed boundary $\partial\mathcal{M}_\epsilon$ by the function $\epsilon s(y)$ with ϵ very small and call the resulting manifold $\mathcal{M}_\epsilon$. Then, to order ϵ, the perturbative formulation of the problem reads as follows,

$$\Delta\psi_\alpha = \alpha^2\psi_\alpha, \quad \psi_\alpha|_{\partial\mathcal{M}_\epsilon} = 0,$$

where the initial ansatz for the eigenfunctions and eigenvalues is given by:

$$\psi_\alpha = \phi_\lambda + \epsilon\phi'_\alpha, \quad \alpha^2 = \lambda^2 + \epsilon\eta_\alpha.$$

The perturbation of the eigenvalues, η_α, is determined by:

$$\eta_\alpha \;=\; \int_{\partial\mathcal{M}_\epsilon} \phi'_\alpha \partial_n \phi^*_\lambda - \int_{\partial\mathcal{M}_\epsilon} \phi^*_\lambda \partial_n \phi'$$

with the exterior normal ∂_n; see, for example, [22]. For Dirichlet conditions one can use the identity $\phi'|_{\partial\mathcal{M}_\epsilon} = -\frac{1}{\epsilon}\phi_\lambda|_{\partial\mathcal{M}_\epsilon}$ together with the expansion

$$\begin{aligned} \phi_\lambda|_{\partial\mathcal{M}_\epsilon} &= \phi_\lambda|_{\partial\mathcal{M}} - \epsilon s(y)\partial_n\phi_\lambda|_{\partial\mathcal{M}} + \ldots \\ &= -\epsilon s(y)\partial_n\phi_\lambda|_{\partial\mathcal{M}} + \ldots \text{ to see} \qquad (9) \\ \eta_\alpha &= -\tfrac{1}{\epsilon}\int_{\partial\mathcal{M}_\epsilon} \phi_\lambda\partial_n\phi^*_\lambda = -\int_{\partial\mathcal{M}_\epsilon} \phi^*_\lambda\partial_n\phi' \int_{\partial\mathcal{M}} s(y)|\partial_n\phi_\lambda|^2 dy. \qquad (10) \end{aligned}$$

It is important to note that the expansion (9) is well defined for the Dirichlet and Neumann eigenfunctions (8).

In the case of degenerate eigenvalues, which is needed here, the situation is slightly more complicated. Let j index the degeneracy. In this case one can obtain the secular equation

$$\sum_j c_{ij}(\eta^i_\alpha\delta_{kj} + B^D_{kj}) = 0, \text{ with} \qquad (11)$$

$$B^D_{kj} = -\int_{\partial\mathcal{M}}(\partial_n\phi^{k*}_\lambda)s(y)(\partial_n\phi^j_\lambda). \qquad (12)$$

Similarly, when considering Neumann conditions and when perturbing the shape of the boundary, the equation analogous to (11) becomes

$$\begin{aligned} &\sum_j c_{ij}(\eta^i_\alpha\delta_{kj} + B^N_{kj}) = 0, \text{ with} \\ &B^N_{kj} = \int_{\partial\mathcal{M}} \phi^{k*}_\lambda s(y)(\partial^2_n\phi^j_\lambda). \qquad (13) \end{aligned}$$

Some of these formulae are implicit in the work of Fröhlich, [8], but can be traced back to Rayleigh, [28]. The extensive discussion in Morse and Feshbach, [22], contains all that one needs. A more mathematical treatment is given by Garabedian and Schiffer, [9] Chap.V, based on Green's theorem and Hadamard's formula.

We apply these developments to the hemisphere. It seems natural to displace the entire boundary by an amount, say ϵ, perpendicular to the equator, *i.e.* the rim, thus making the new manifold a cap. Geometry shows that the extrinsic curvature, $L^{\partial\mathcal{M}}$, of the perturbed boundary equals ϵ. Then the relevant integrals for the eigenvalue perturbations are,

$$\begin{aligned} B^D_{\mu\mu'} &= -2\mathcal{N}_1^2\mu\mu' L^{\partial\mathcal{M}} \int_0^\pi \frac{d\theta}{\sin^2\theta}\, P_l^\mu(\cos\theta)\, P_l^{\mu'}(\cos\theta), \text{ and} \\ B^N_{\mu\mu'} &= -2\mathcal{N}_2^2\mu'^{\,2} L^{\partial\mathcal{M}} \int_0^\pi \frac{d\theta}{\sin^2\theta}\, P_l^\mu(\cos\theta)\, P_l^{\mu'}(\cos\theta). \end{aligned} \tag{14}$$

The behaviour of the Legendre functions for $\theta \to 0, \pi$ shows that these integrals exist and, although an explicit evaluation is tedious (they are surprisingly not listed in standard references like [1, 13]), in principle this determines the eigenvalues to order ϵ and undoubtedly would reproduce the correct leading heat kernel expansion. We have not pursued this calculational check.

It seems reasonable to apply the same perturbative approach to the N/D problem. In this case the N and D parts contribute additively to the secular equation,

$$\sum_j c_{ij}(\eta^i_\alpha \delta_{kj} + B^D_{kj} + B^N_{kj}) = 0,$$

where the definitions (12) and (13) still hold but involving the eigenfunctions of the N/D problem. As one soon realizes, all integrals exist, *except* the ones with $\mu = \mu' = -1/2$. The reason may be found in the use of (9) which *cannot* be applied for these modes because it leads to divergences at the edges of the manifold. To avoid the use of (9) we revert to (10) and evaluate just *these* awkward modes on the perturbed boundary, $\partial\mathcal{M}_\epsilon$, directly.

We return to Dirichlet conditions, where everything is well defined, to illustrate the situation. The boundary $\partial\mathcal{M}_\epsilon$ can be parametrised by noting that along it, $y = \epsilon = \sin\theta\sin\varphi$, *i.e.*

$$\varphi = \sin^{-1}\left(\frac{\epsilon}{\sin\theta}\right), \quad x \geq 0, \text{ and } \varphi = \pi - \sin^{-1}\left(\frac{\epsilon}{\sin\theta}\right), \quad x \leq 0.$$

To leading order in ϵ, the geometrical quantities (normal derivative and volume element) on $\partial\mathcal{M}_\epsilon$ agree with those on $\partial\mathcal{M}$ and, up to irrelevant corrections, one finds

$$B^D_{\mu\mu'} = -2\mathcal{N}_1^2\mu' L^{\partial M}\frac{1}{\epsilon}\int_\epsilon^{\pi-\epsilon}\frac{d\theta}{\sin\theta}P_l^\mu(\cos\theta)P_l^{\mu'}(\cos\theta)\times \sin\left[\mu\sin^{-1}\frac{\epsilon}{\sin\theta}\right]\cos\left[\mu'\sin^{-1}\frac{\epsilon}{\sin\theta}\right]. \quad (15)$$

To the relevant order, the integration limits can be set to 0 and π and comparison of (14) with (15) shows that the expansion with respect to ϵ of the eigenfunctions evaluated at $\partial\mathcal{M}_\epsilon$ leads to the occurrence of a factor $\epsilon/\sin\theta$ to give agreement with the perturbation form.

Turning to the N/D problem, we are therefore led to consider integrals of the type

$$\int_\epsilon^{\pi-\epsilon}\frac{d\theta}{\sin^2\theta}P_l^{-\mu}(\cos\theta)P_l^{-\mu'}(\cos\theta)$$

which are well defined in the limit $\epsilon\to 0$ for all values of μ,μ' *except* $\mu=\mu'=1/2$. For these "critical subspaces", using the explicit Gegenbauer representation [13],

$$P^{-1/2}_{\nu-1/2}(\cos\theta) = \sqrt{\frac{2}{\pi\sin\theta}}\frac{\sin(\nu\theta)}{\nu},$$

the relevant integrals have the form

$$\int_\epsilon^{\pi-\epsilon} d\theta\frac{\sin^2[(n+1)\theta]}{\sin^3\theta},$$

which behaves like $\log\epsilon = \log L^{\partial M}$ as $\epsilon\to 0$. All other eigenfunctions yield an $\mathcal{O}(\epsilon)$ term to leading order and will not change this log behaviour. These remarks suggest the existence of a term $L^{\partial M}\log L^{\partial M}$ in the heat trace expansion which is an indirect indication, via dimensional arguments, of the appearance of $\log t$ terms as well (see § 5).

Thinking about higher order perturbation theory, it is expected that modes which are differentiable only $(k-1)$ times, $k\in\mathbb{N}$, lead to the occurrence of $\epsilon^k\log\epsilon$ with associated $\log t$ terms in the heat trace expansion.

We stress that, for the perturbed geometry, the extrinsic curvature $L^{\partial\mathcal{M}}$ does not vanish at the edge and this is the cause of the trouble. When the boundary perturbation, $s(y)$, vanishes at the edges, the perturbation is well defined and we expect the standard trace expansions to hold.

5 Conclusions

We have shown that if there is an asymptotic expansion of the heat trace for the N/D problem, then it is not as simple as in the standard setting. It is possible that $\log t$ terms enter, the generic behaviour for singular situations. There is one setting where such terms are known to arise. If instead of local boundary conditions, spectral conditions are imposed, one has a partial asymptotic expansion of the form,

$$a(D,\mathcal{B})(t) = \sum_{n<m} a_n(D,\mathcal{B})t^{(n-m)/2} + O(t^{-\frac{1}{8}}).$$

Again the invariants are locally computable and we refer to [7, 12] for formulae if $n \leq 3$. However, the complete asymptotic expansion involves non-local and log terms [17, 18]. Thus perhaps Conjecture 3 should be replaced by an asymptotic expansion of the form

$$a(D,\mathcal{B})(t) \sim \textstyle\sum_{n\geq 0} \Big(\alpha_n(D,\mathcal{B}) \log t + a_n(D,\mathcal{B})\Big) t^{(n-m)/2}$$

where the leading term $\alpha_n(D,\mathcal{B}) = \int_\Sigma \alpha_n^\Sigma(z,D,\mathcal{B})dz$ is locally computable and where the difference

$$a_n(D,\mathcal{B}) - \textstyle\int_M a_n(x,D)dx - \int_{C_D} a_n^-(y,D,\mathcal{B})dy - \int_{C_N} a_n^+(y,D,\mathcal{B})dy$$

is a non-local invariant determined by the behavior of D and $\mathcal{B}$ near Σ. As we have argued in Section 4, $\log t$ terms may occur to compensate the $\log L^{\partial M}$ terms present in the perturbed hemisphere example. Further study of the heat trace asymptotics of the D/N problem seems indicated.

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