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ON THE Θ-FUNCTION OF A RIEMANNIAN MANIFOLD WITH BOUNDARY

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ABSTRACT. Let Ω be a compact Riemannian manifold of dimension n with smooth boundary. Let $\lambda_1 < \lambda_2 \le \cdots$ be the eigenvalues of the Laplace-Beltrami operator with the boundary condition $[\partial/\partial n + \gamma]\phi = 0$. The associated Θ-function $\Theta_\gamma(t) = \sum_{n=1}^{\infty} \exp[-\lambda_n t]$ has an asymptotic expansion of the form

$$(4\pi t)^{n/2}\Theta_\gamma(t) = a_0 + a_1 t^{1/2} + a_2 t + a_3 t^{3/2} + a_4 t^2 + \cdots .$$

The values of a_0, a_1 are well known. We compute the coefficients a_2 and a_3 in terms of geometric invariants associated with the manifold by studying the parametrix expansion of the heat kernel $p(t, x, y)$ near the boundary. Our method is a significant refinement and improvement of the method used in [McKean-Singer, J. Differential Geometry **1** (1969), 43–69].

1. INTRODUCTION

The present work is devoted to the study of the asymptotic expansion of the so-called Θ-function of the third boundary value problem under the general setting of a Riemannian manifold with smooth boundary. The Θ-function is defined as follows. Let Ω be a compact Riemannian manifold of dimension n with smooth boundary. The Laplace-Beltrami operator is denoted by Δ. Let γ be a smooth function defined on the boundary $\partial\Omega$. We do not assume that γ is strictly positive.

Consider the following eigenvalue problem

$$\begin{cases} \Delta\phi + \lambda\phi = 0, & \text{on } \Omega, \\ \left[\frac{\partial}{\partial n} + \gamma\right]\phi = 0, & \text{on } \partial\Omega. \end{cases}$$

(n denotes the *outward* unit normal vector at the boundary). Let $\{\lambda_n, \phi_n\}$, $n = 1, 2, \ldots$, be the normalized eigenpairs. The Θ-function of the boundary value problem is by definition

$$\Theta_\gamma(t) = \sum_{n=1}^{\infty} e^{-\lambda_n t}.$$

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This function is very important in the study of asymptotic properties of the eigenvalue distribution. In the simplest case when Ω is the circle of radius one, $\Theta_\gamma(t)$ is the famous Jacobi θ-function

$$\theta(t) = \sum_{n=-\infty}^{\infty} e^{-n^2 t}.$$

For $\theta(t)$, we have the Jacobi inversion formula

$$\theta(t) = \sqrt{\frac{\pi}{t}}\theta\left(\frac{\pi^2}{t}\right),$$

from which it follows that $\sqrt{4\pi t}\theta(t) = 2\pi + O(t^k)$ for any $k > 0$. This is the simplest case of the asymptotic formula we still study in this paper.

Abstract analysis shows that $\Theta_\gamma(t)$ has an *asymptotic* expansion of the form (see [G]):

$$(1.1) \qquad (4\pi t)^{n/2}\Theta_\gamma(t) = a_0 + a_1 t^{1/2} + a_2 t + a_3 t^{3/2} + a_4 t^2 + \cdots .$$

In the case of a manifold without boundary, all terms with fractional powers of t disappear.

The study of the behavior of the Θ-function as $t \to 0$ was initiated by the work of Kac [K]. The central question there was whether the eigenvalues of an Euclidean domain determines the domain uniquely. Kac studied this problem by obtaining explicit formulas for the coefficients a_i in terms of geometric invariants of the domain. For an Euclidean domain, Kac computed the first two terms under the Dirichlet boundary condition $(\gamma = \infty)$:

$$a_0 = |\Omega|, \qquad a_1 = -\frac{\sqrt{\pi}}{2}|\partial\Omega|,$$

and went on to conclude that the eigenvalues determine the volume and the boundary area of an Euclidean domain. Since then computations have been carried out for more general domains (e.g., on a Riemannian manifold) and for more coefficients. The most significant work in this direction is [MS], in which the coefficient a_2 is computed for a general Riemannian manifold under the Dirichlet or the Neumann boundary condition:

$$a_2 = \frac{1}{6}\int_\Omega K(x)\,dx - \frac{1}{3}\int_{\partial\Omega} M(z)\sigma(dz),$$

where $K(x)$ is the scalar curvature of Ω at x and $M(z)$ is the mean curvature of the boundary $\partial\Omega$ at z. In the present work, we will carry out the computations for a_2 and a_3 in the most general situation stated at the beginning of this section.

The chief reason that $\Theta_\gamma(t)$ can be studied analytically is its connection with the heat kernel $p_\gamma(t, x, y)$. By definition, $p_\gamma(t, x, y)$ is the fundamental solution of the heat equation with the boundary condition $[\partial/\partial n + \gamma]\phi = 0$, i.e., it is the unique nonnegative smooth function defined on $(0, \infty) \times \overline{\Omega} \times \overline{\Omega}$ which satisfies the following two properties:

(i) For fixed $x \in \overline{\Omega}$, it satisfies the heat equation in t, y:

$$\frac{\partial}{\partial t}p_\gamma(t, x, y) = \Delta_y p_\gamma(t, x, y),$$

and the boundary condition

$$\left[\frac{\partial}{\partial n_y} + \gamma(y)\right] p_\gamma(t, x, y) = 0$$

(subscript y means that the derivatives are taken in y variables);

(ii) For any function f continuous on $\overline{\Omega}$,

$$\lim_{t\to 0} \int_\Omega f(y)p(t, x, y)\, dy = f(x).$$

It is well known that the heat kernel has the following expansion in terms of the eigenvalues and the eigenfunctions (Mercer's expansion):

$$p_\gamma(t, x, y) = \sum_{n=1}^{\infty} e^{-\lambda_n t}\phi_n(x)\phi_n(y).$$

Setting $x = y$ and integrating over Ω, we obtain the formula

$$\Theta_\gamma(t) = \int_\Omega p_\gamma(t, x, x)\, dx. \tag{1.2}$$

Thus $\Theta_\gamma(t)$ can be studied by constructing good approximations of the heat kernel.

Let us mention some previously known results before stating our main theorems. As mentioned earlier, a_0, a_1 were computed in [K] for Euclidean domains, and a_2 for the Dirichlet and the Neumann cases were computed in [MS] for compact Riemannian manifolds with smooth boundary. The formula for a_2 appeared in [KCD]. The coefficient a_3 was computed in [P] for a two dimensional, strictly convex Euclidean domain

$$a_3 = \begin{cases} \frac{1}{64}\sqrt{\pi}\int_{\partial\Omega} k(z)^2\sigma(dz), & \text{with Dirichlet boundary condition},\\ \frac{7}{64}\sqrt{\pi}\int_{\partial\Omega} k(z)^2\sigma(dz), & \text{with Neumann boundary condition},\end{cases} \tag{1.3}$$

where $k(z)$ is the curvature of the boundary $\partial\Omega$ and $\sigma(dz)$ is the arclength. Much later, apparently unaware of [P], Louchard [L] used a probabilistic method and recomputed a_2 under the same conditions on the domain. Waechter [W] extended Pleijel's method and computed a_3 for three dimensional, strictly convex Euclidean domain with the Dirichlet boundary condition

$$a_3 = \frac{1}{64}\sqrt{\pi}\int_{\partial\Omega} [k_1(z) - k_2(z)]^2\sigma(dz), \tag{1.4}$$

where $k_1(z)$, $k_2(z)$ are the two principal curvatures of the boundary surface at point z.

The formula for the coefficient a_3 in the case where the ambient space is flat appeared in [KCD] without proof. Our formula for a_3 and a sketch of the proof was announced in [H]. We are happy to acknowledge the recent independent work of Gilkey and Branson [GB] where a_3 and a_4 are computed using a different method.

We now state our result. As before, Ω is a compact Riemannian manifold with smooth boundary $\partial\Omega$. We will use H to denote the second fundamental form of the boundary $\partial\Omega$. The scalar curvature of Ω at x is denoted by $K(x)$. The scalar curvature of $\partial\Omega$ (equipped with the induced metric) at z is denoted by $K^{\partial\Omega}(z)$. The Ricci curvature of Ω at z in the normal direction n of the boundary is denoted by $\mathrm{Ric}(n)(z)$.

Theorem 1. *The first four coefficients in the asymptotic expansion of the* Θ-*function with the boundary condition* $[\partial/\partial n+\gamma]\phi=0$ *are*

$$a_0=|\Omega|,$$
$$a_1=\frac{\sqrt{\pi}}{2}|\partial\Omega|,$$
$$a_2=\frac{1}{6}\int_\Omega K(x)\,dx-\frac{1}{3}\int_{\partial\Omega}[\mathrm{tr}\ H(z)+6\gamma(z)]\sigma(dz),$$
$$a_3=\sqrt{\pi}\int_{\partial\Omega}\left[\frac{1}{12}K^{\partial\Omega}(z)-\frac{37}{192}(\mathrm{tr}\ H(z))^2+\frac{29}{96}\mathrm{tr}\ H(z)^2+\frac{1}{8}\mathrm{Ric}(n)(z)\right]\sigma(dz)$$
$$+\sqrt{\pi}\int_{\partial\Omega}\left[\frac{1}{2}\gamma(z)\mathrm{tr}\ H(z)+\gamma(z)^2\right]\sigma(dz).$$

The coefficients for the case of the Neumann condition are obtained by setting $\gamma\equiv 0$ *in these formulas.* □

Theorem 2. *The first four coefficients in the asymptotic expansion of the* Θ-*function with the Dirichlet boundary condition are*

$$a_0=|\Omega|,$$
$$a_1=-\frac{\sqrt{\pi}}{2}|\partial\Omega|,$$
$$a_2=\frac{1}{6}\int_\Omega K(x)\,dx-\frac{1}{3}\int_{\partial\Omega}\mathrm{tr}\ H(z)\sigma(dz),$$
$$a_3=\sqrt{\pi}\int_{\partial\Omega}\left[-\frac{1}{12}K^{\partial\Omega}(z)+\frac{13}{192}(\mathrm{tr}\ H(z))^2-\frac{5}{96}\mathrm{tr}\ H^2(z)-\frac{1}{8}\mathrm{Ric}(n)(z)\right]\sigma(dz).$$

□

Remark. For a smooth domain in R^3 we have

$$K^{\partial\Omega}=2k_1k_2,\quad (\text{Gauss' } \textit{Theorema egregium}),$$
$$\mathrm{Ric}(n)=0,\qquad \mathrm{tr}\ H=-k_1-k_2,\qquad \mathrm{tr}\ H^2=k_1^2+k_2^2.$$

We can thus recover (1.4) from the general formula in Theorem 2. In the Neumann case, we have from Theorem 1

$$a_3=\frac{7}{64}\sqrt{\pi}\int_{\partial\Omega}[k_1(z)-k_2(z)]^2\sigma(dz).$$

The general plan of the paper is as follows. The first step, carried out in §2, is to reduce the general case $\gamma\neq 0$ to the Neumann case $\gamma=0$. After such reduction we only have two cases to consider, the Dirichlet case and the Neumann case. The heat kernel in these two cases will be denoted by $p_D(t,x,y)$ and $p_N(t,x,y)$ respectively. The two cases being similar, we will concentrate on the Neumann case. The method we will use to compute the asymptotic expansion of

$$\Theta_N(t)=\int_\Omega p_N(t,x,x)\,dx$$

follows in broad outline the parametrix method in [MS]. However, a brute force attempt to push the computation there to one more term in the asymptotic expansion can easily be frustrated by an insurmountable amount of computation can be kept within a workable limit.

In order to obtain the desired precision in our calculation, we need to compute the first few terms of the Taylor expansion of the metric matrix in a suitably chosen coordinate system near the boundary. This computation is done in §3. At the beginning of §4 we will use the localization principle (stated in §7) to reduce the computation to a thin collar at the boundary. We then construct the heat kernel near the boundary and make some necessary estimates to set up for the computations in the next section. Lengthy computations are carried out in §5. From the expansion of the metric in §3 and the computations in §5 we conclude that the coefficient a_3 has to have the form

$$a_3 = \int_{\partial\Omega} a_3(z)\sigma(dz)$$

where $a_3(z)$ is a linear combination of the following terms

$$a_3(z) = AK^{\partial\Omega}(z) + B\mathrm{Ric}(n)(z) + C(\operatorname{tr} H(z))^2 + D\operatorname{tr} H(z)^2.$$

The work in §5 gives explicitly the values of A and B but not those of C and D. Determination of C, D by direct computation involves calculating a large number of definite integrals. To avoid these calculations, we show in §6 that A, B, C, D are universal constants, i.e., *they are independent of the dimension of the manifold*. This important observation allows us to determine the two remaining coefficients C, D by the explicit results of Euclidean balls of dimensions 2 and 3. Fortunately, the values of a_3 in these two special cases are available. In dimension two, it can be read off from (1.3) above. It turns out that for a ball of dimension 3, a_3 is equal to zero for both the Dirichlet case (see (1.4) above) and the Neumann case. The computation of the latter case was carried out in [Z]. Having known a_3 for these two cases, we can determine C, D in the general case by solving two linear equations.

The last section (§7) contains a discussion of the localization principle of the heat kernel, which are used on several occasions in the paper.

Throughout this paper, letters c, α, β, γ, δ, with or without subscripts, and t_0 denote constants whose values are unimportant and may change from one appearance to another.

2. Reduction to the Neumann case

As before $p_N(t, x, y)$ denotes the heat kernel on Ω with the Neumann boundary condition. The impedance function γ is assumed to be smooth on $\partial\Omega$.

Proposition 3. *The heat kernel $p_\gamma(t, x, y)$ can be expressed as an infinite series*

$$p_\gamma(t, x, y) = \sum_{m=0}^{\infty}(-1)^m F_m(t, x, y), \tag{2.1}$$

where

$$\begin{aligned} &F_0(t, x, y) = p_N(t, x, y), \\ &F_m(t, x, y) = \int_0^t ds \int_{\partial\Omega} p_N(t-s, x, z)\gamma(z)F_{m-1}(s, z, y)\sigma(dz). \end{aligned} \tag{2.2}$$

Proof. The boundary condition for $p_\gamma(t, x, y)$ can be written as

$$\partial p_\gamma(t, x, y)/\partial n_y = -\gamma(y)p_\gamma(t, x, y).$$

Thus by the superposition principle of the heat equation, $p_\gamma(t, x, y)$ is the sum of the solutions of two initial-boundary value problems of the heat equation: (i) $p_N(t, x, y)$ with initial value δ_x (the Dirac delta function at x) and the boundary condition $\partial p_N(t, x, y)/\partial n_y = 0$; and (ii) $g(t, x, y)$ with initial value zero and the boundary condition $\partial g(t, x, y)/\partial n_y = -\gamma(y)p_\gamma(t, x, y)$. The solution $g(t, x, y)$ can be expressed as

$$g(t, x, y) = -\int_0^t ds \int_{\partial\Omega} p_N(t-s, x, z)\gamma(z)p_\gamma(s, z, y)\sigma(dz).$$

Hence we have an integral equation for $p_\gamma(t, x, y)$:

$$p_\gamma(t, x, y) = p_N(t, x, y) - \int_0^t ds \int_{\partial\Omega} p_N(t-s, x, z)\gamma(z)p_\gamma(s, z, y)\sigma(dz).$$

We obtain the series for $p_\gamma(t, x, y)$ by iteration. □

We will often use the following simple estimate for the Neumann heat kernel: There exist positive constant t_0, c_1 such that for all $t < t_0$, $(x, y) \in \overline{\Omega} \times \overline{\Omega}$,

$$p_N(t, x, y) \le c_1 t^{-n/2} e^{-d(x, y)^2/c_1 t}. \tag{2.3}$$

This estimate can be verified by the parametrix method, see (4.12) below. Note that in this estimate, the Riemannian distance $d(x, y)$ can be replaced by any distance function $D(x, y)$ which is compatible with the Riemannian distance in the sense that there exists a constant $\lambda > 0$ such that $\lambda^{-1}D(\cdot, \cdot) \le d(\cdot, \cdot) \le \lambda D(\cdot, \cdot)$. We often replace d by the Euclidean distance of a local cartesian coordinate system.

We claim

$$(4\pi t)^{n/2} \sum_{m=3}^{\infty} \int_\Omega |F_m(t, x, x)|\, dx = O(t^2). \tag{2.4}$$

The proof runs as follows. We first verify (2.4) under the assumptions that Ω is the half-space $R^n_+ = \{x = (x^1, \dots, x^n) : x^1 > 0\}$ and that the metric is the usual Euclidean metric outside a neighborhood of the origin. Under these assumptions, we may replace $d(x, y)$ in (2.3) by the Euclidean distance $|x-y|$. Furthermore (2.3) holds globally for all x, y (see (4.11) and (4.12)). We now use the convolution property of the Gaussian kernel to verify by induction that $F_m(t, x, y)$ has an estimate of the following form:

$$|F_m(t, x, y)| \le c_2 c_3^m \Gamma\left(\frac{m+1}{2}\right)^{-1} t^{(m-n)/2} e^{-|x-y|^2/c_1 t}.$$

Summing over m and using (2.1), we see that there exist positive constants c_4, t_0 such that for all $t < t_0$ and all x, y,

$$p_\gamma(t, x, y) \le c_4 t^{-n/2} e^{-|x-y|^2/c_1 t}. \tag{2.5}$$

Let $G_m(t, x, y)$ be the function $(-1)^m F_m(t, x, y)$ under the boundary function $\gamma \equiv -\|\gamma\|_\infty$. By the recursive relation (2.2) of $G_m(t, x, y)$,

$$\begin{aligned}\sum_{m=2}^{\infty} G_m(t, x, y) \le \|\gamma\|_\infty^2 \int_0^t ds_1 \int_{\partial\Omega} p_N(t-s_1, x, z_1)\sigma(dz_1) \\ \times \int_0^{s_1} ds_2 \int_{\partial\Omega} p_N(s_1-s_2, z_1, z_2) \sum_{m=0}^{\infty} G_m(s_2, z_2, y)\sigma(dz_2).\end{aligned} \tag{2.6}$$

But it is clear from (2.1) and (2.2) that

$$\sum_{m=0}^{\infty} G_m(s, z, y) \le p_{-\|\gamma\|_\infty}(s, z, y).$$

Hence the right-hand side of (2.6) can be estimated by the Gaussian type upper bounds (2.3) and (2.5) of the heat kernels $p_N(t, x, y)$ and $p_{-\|\gamma\|_\infty}(t, x, y)$ and we obtain

$$\sum_{m=2}^{\infty} G_m(t, x, y) \le c_6 t^{(2-n)/2} e^{-d(x,y)^2/c_7 t}. \tag{2.7}$$

From the recursive relation of $G_m(t, x, y)$ again, we have

$$\begin{aligned}\int_\Omega G_m(t, x, x)\, dx = \|\gamma\|_\infty^2 \int_0^t (t-u)du \int_{\partial\Omega} \sigma(dy) \\ \times \int_{\partial\Omega} p_N(t-u, y, z) G_{m-2}(u, z, y)\sigma(dz).\end{aligned}$$

Hence

$$\begin{aligned}\int_\Omega G_m(t, x, x)\, dx \le \|\gamma\|_\infty^2 t \int_0^t du \int_{\partial\Omega} \sigma(dy) \\ \times \int_{\partial\Omega} p_N(t-u, y, z) G_{m-1}(u, z, y)\sigma(dz) \\ = \|\gamma\|_\infty t \int_{\partial\Omega} G_{m-1}(t, y, y)\sigma(dy).\end{aligned} \tag{2.8}$$

Summing over m from 3 to infinity and using (2.7), we obtain (2.4) with $F_m(t, x, x)$ replaced by $G_m(t, x, x)$. (2.4) now follows immediately from the inequality $|F_m(t, x, y)| \le G_m(t, x, y)$. Thus (2.4) is proved for the case of Euclidean half-space. In the general case of a compact manifold with boundary, the localization principle in §7 shows there exists a $\delta > 0$ such that (2.5) holds for all x, y on Ω satisfying $d(x, y) \le \delta$. This fact can then be used together with the localization principle again to show via (2.6) that (2.7) holds under the same condition on x and y. This suffices for (2.8) since we only need (2.7) for $x = y$. The proof of (2.4) is completed. □

Now we have from (1.2), (2.1), and (2.4)

$$\Theta_\gamma(t) = \Theta_N(t) + \int_\Omega F_1(t, x, x)\, dx + \int_\Omega F_2(t, x, x)\, dx + O(t^2). \tag{2.9}$$

The difficult term $\Theta_N(t)$ will be dealt with in §§3 and 6. In the rest of this section, we study the integrals of $F_i(t, x, x)$, $i = 1, 2$, over Ω. For this purpose we need

Proposition 4. *As* $t \to 0$, *we have uniformly in* $z \in \partial\Omega$:

$$(4\pi t)^{n/2} p_N(t, z, z) = 2[1 - \tfrac{1}{4}\mathrm{tr}\, H(z)\sqrt{\pi t}] + O(t).$$

Recall that tr $H(z)$ *is the mean curvature of the boundary.*

We will prove this proposition at the end of §5.

Lemma 5. *We have as* $t \to 0$,

$$(4\pi t)^{n/2} \int_\Omega F_1(t, x, x)\, dx$$
$$= 2t \int_{\partial\Omega} \gamma(z)\sigma(dz) - \frac{1}{2}\sqrt{\pi} t^{3/2} \int_{\partial\Omega} \gamma(z) \mathrm{tr}\, H(z)\sigma(dz) + O(t^2),$$

and

$$(4\pi t)^{n/2} \int_\Omega F_2(t, x, x)\, dx = \sqrt{\pi} t^{3/2} \int_{\partial\Omega} \gamma(z)^2 \sigma(dz) + O(t^2).$$

Proof. The definition of $F_1(t, x, x)$ and the Chapman-Kolmogorov equation of the heat kernel imply

$$\int_\Omega F_1(t, x, x)\, dx = t \int_{\partial\Omega} p_N(t, z, z)\gamma(z)\sigma(dz).$$

The first assertion follows immediately from the above identity and Proposition 4.

To prove the second assertion, we use

$$\int_\Omega F_2(t, x, x)\, dx = \int_0^t (t-u)du \int_{\partial\Omega} \gamma(z)\sigma(dz)$$
$$\times \int_{\partial\Omega} p_N(t-u, z, y)\gamma(y)p_N(u, y, z)\sigma(dy).$$

We replace $\gamma(y)$ in the above integral by $\gamma(z)+O(d(z, y))$ and split the integral into two integrals accordingly. Using the upper bound for the heat kernel (2.3) we find that

$$\int_{\partial\Omega} d(z, y)p_N(t-u, y, z)p_N(u, z, y)\sigma(dy)$$
$$\le c_1[u(t-u)]^{-n/2} \int_{R^{n-1}} |y| e^{-c_2|y|^2 t/u(t-u)}\, dy.$$

The last integral is bounded by $c_3 t^{-n/2}$. Hence

$$\int_\Omega F_2(t, x, x)\, dx = \int_{\partial\Omega} \gamma(z)^2 g(t, z)\sigma(dz) + O(t^{(4-n)/2}),$$

where

$$g(t, z) = \int_0^t (t-u)du \int_{\partial\Omega} p_N(t-u, y, z)p_N(u, z, y)\sigma(dy).$$

The right-hand side can be computed by taking the first term in the series expansion (4.1) of the heat kernels $p_N(t-u, y, z) = 2q(t-u, y, z)$ and $p_N(u, z, y) = 2q(u, z, y)$ (Note that $z^* = z$ if $z \in \partial\Omega$.) The explicit computation can be carried out with the help of a suitably chosen local coordinate system (see §3) and the localization principle. We leave the details of this computation to the interested reader and we content ourselves with the statement that the leading term of $g(t, z)$ is equal to the same integral in the Euclidean space, i.e.,

$$\begin{aligned}(4\pi t)^{n/2} g(t, z) &= 4\int_0^t \left[\frac{1}{4\pi}\frac{t}{u(t-u)}\right]^{n/2} (t-u)\,du \\ &\quad \times \int_{R^{n-1}} \exp\left\{-\frac{|z-y|^2}{4(t-u)} - \frac{|y-z|^2}{4u}\right\} dy + O(t^2) \\ &= \sqrt{\frac{4t}{\pi}} \int_0^t \sqrt{\frac{t-u}{u}}\, du + O(t^2) \\ &= \sqrt{\pi} t^{3/2} + O(t^2).\end{aligned}$$

This yields the second assertion. □

Up to now all terms in Theorem 1 and involving γ have been accounted for. In the rest of this paper, we take up the asymptotic expansions of $\Theta_D(t)$ and $\Theta_N(t)$.

3. Calculations concerning the Riemannian metric near the boundary

In the next section we will construct the heat kernel $p_D(t, x, y)$ and $p_N(t, x, y)$ by the parametrix method. In order to obtain enough terms in the expansion of the heat kernel, we need to know the Taylor expansion of the metric matrix in a suitably chosen coordinate system near the boundary. This section is devoted to the development of such expansion.

We will work in a neighborhood of a fixed point on the boundary. Take this point to be the origin O of our local coordinates $x = (x^1, \tilde{x}) = (x^1, x^2, \dots, x^n)$. The first coordinate x^1 is defined to be $d(x, \partial\Omega)$, the Riemannian distance from point x to the boundary. The remaining coordinates $\tilde{x} = (x^2, x^3, \dots, x^n)$ are defined to be the normal cartesian coordinates of $\partial\Omega$ (as a Riemannian manifold with the induced metric) in a neighborhood of the origin O, i.e., $\tilde{x}$ is the image (by the exponential map at O) of the cartesian coordinates in the tangent plane of $\partial\Omega$ at O. In the next section, we will consider the double of Ω. In such case, the metric matrix is extended to the region $x^1 < 0$ by setting $g(x^1, \tilde{x}) = g(-x^1, \tilde{x})$. In this section we assume that g has been extended as such.

The advantage of choosing the coordinate system we have just defined is that the quantities that appear in the general formula of a_3 are all singled out by the expansion of the metric matrix in these coordinates. See Proposition 6 below.

In the statement of the next proposition and the rest of the paper, we will use the following conventions: (1) the second fundamental form matrix $H = \{H_{ij}, 2 \le i, j \le n\}$ is an $(n-1) \times (n-1)$ matrix. We extend it to an $n \times n$ matrix by setting $H_{1j} = 0$ for $j = 1, \dots, n$; (2) without stating the contrary, repeated indices are summed over from 2 to n, *not* from 1 to n.

Proposition 6. *Let O be a point on the boundary $\partial\Omega$. In the local coordinates described above, the Riemannian metric matrix $g = (g_{ij}(x))$ has the following expansion in a neighborhood of O.*

(a) $g_{1j}(x) = \delta_{1j}$ *for* $j = 1, \dots, n$;
(b) *for* $2 \le i, j \le n$,

$$g_{ij}(x) = \delta_{ij} + 2H_{ij}|x^1| + (-R_{1i1j} + (H^2)_{ij})|x^1|^2 + 2\partial_k H_{ij}|x^1|x^k - \tfrac{1}{3}R^{\partial\Omega}_{ikjl}x^k x^l + O(|x|^3).$$

Here $H = \{H_{ij}\}$ *is the matrix of the second fundamental form of the boundary,* R_{ikjl} *are the components of the curvature tensors of* Ω, *and* $R^{\partial\Omega}_{ikjl}$ *are the components of the curvature tensor of* $\partial\Omega$ *with the induced metric. All quantities are evaluated at* O.

Proof. First of all, since the coordinate line $\tilde{x} =$ const. is a geodesic perpendicular $\partial\Omega$, we have $g_{1j}(0, \tilde{x}) = \delta_{1j}$ for all $\tilde{x} \in \partial\Omega$, and $\nabla_1\partial_1 = 0$ (the equation of geodesics). Hence

$$\partial_1 g_{1j}(x) = \langle \partial_1, \nabla_1\partial_j\rangle = \langle \partial_1, \nabla_j\partial_1\rangle = \tfrac{1}{2}\nabla_j\langle \partial_1, \partial_1\rangle = 0.$$

($\langle\cdot, \cdot\rangle$ denotes the inner product in the Riemannian metric.) It follows that $g_{1j}(x) \equiv \delta_{1j}$. This proves part (a).

The second fundamental form matrix H_{ij} is defined by

$$H_{ij} = H(\partial_i, \partial_j) = -\langle \nabla_i\partial_j, \partial_1\rangle.$$

(∇_i denotes covariant derivative along $\partial_i = \partial/\partial x^i$. Note that ∂_1 is the inward unit normal vector.) Now assume that neither i nor j is equal to 1. We have

$$\begin{aligned}\partial_1 g_{ij} &= \langle \nabla_1\partial_i, \partial_j\rangle + \langle \partial_i, \nabla_1\partial_j\rangle = \langle \nabla_i\partial_1, \partial_j\rangle + \langle \partial_i, \nabla_j\partial_1\rangle \\ &= \nabla_i\langle \partial_1, \partial_j\rangle - \langle \partial_1, \nabla_i\partial_j\rangle + \nabla_j\langle \partial_i, \partial_1\rangle - \langle \nabla_j\partial_i, \partial_1\rangle \\ &= 2H_{ij}.\end{aligned}$$

This also implies $\partial_k\partial_1 g_{ij} = 2\partial_k H_{ij}$. Next we note that in our coordinates, $R_{j11i} = \langle \nabla_1\nabla_i\partial_1, \partial_j\rangle$. This identity is used in the last step of the following computation:

$$\begin{aligned}\partial_1\partial_1 g_{ij} &= \partial_1\partial_1\langle \partial_i, \partial_j\rangle = \partial_1\langle \nabla_1\partial_i\partial_j\rangle + \partial\langle \partial_i, \nabla_1\partial_j\rangle \\ &= \partial_1\langle \nabla_i\partial_1, \partial_j\rangle + \partial_1\langle \partial_i, \nabla_j\partial_1\rangle \\ &= \langle \nabla_1\nabla_i\partial_1, \partial_j\rangle + \langle \partial_i, \nabla_1\nabla_j\partial_1\rangle + \langle \nabla_i\partial_1, \nabla_j\partial_1\rangle + \langle \nabla_i\partial_1, \nabla_j\partial_1\rangle \\ &= R_{j11i} + R_{i11j} + 2\langle \nabla_i\partial_1, \nabla_j\partial_1\rangle \\ &= -2R_{1i1j} + 2\langle \nabla_i\partial_1, \nabla_j\partial_1\rangle.\end{aligned}$$

We want to express the last term in terms of the second fundamental form matrix H. Because $\langle \partial_l, \partial_1\rangle = 0$ for $2 \le l \le n$, we have $H_{il} = \langle \partial_l, \nabla_i\partial_1\rangle$. Since $\{\partial_1, \dots, \partial_n\}$ form an orthonormal basis at O and $\langle \nabla_i\partial_1, \partial_1\rangle = 0$, we have $\nabla_i\partial_1 = \sum_{l=2}^n H_{il}\partial_l$. Thus

$$\langle \nabla_i\partial_1, \nabla_j\partial_1\rangle = H_{il}H_{jk}\langle \partial_l, \partial_k\rangle = H_{ik}H_{kj}.$$

It follows that

$$\partial_1\partial_1 g_{ij} = -2R_{1i1j} + 2(H^2)_{ij}.$$

The only case left is $\nabla_k\nabla_l g_{ij}$, where none of the four indices is equal to 1. It is a classical result of E. Cartan (see [BGM, p. 97 or CE, pp. 15–16]) that in the normal cartesian coordinates, the metric matrix $g^{\partial\Omega}(\tilde{x}) = g(0, \tilde{x})$ has the expansion

$$g_{ij}(0, \tilde{x}) = \delta_{ij} - \tfrac{1}{3}R^{\partial\Omega}_{ikjl}x^k x^l + O(|\tilde{x}|^3).$$

Part (b) is proved. □

We now use the above expansion of the metric g to compute the first and second derivatives of several functions.

First of all, we compute the first few terms of the Taylor expansion of the volume element

$$J(x) \stackrel{\text{def}}{=} \sqrt{\det g(x)}.$$

For any square matrix, we have

$$\det[I+A] = 1 + \operatorname{tr} A + \tfrac{1}{2}[(\operatorname{tr} A)^2 - \operatorname{tr}(A^2)] + O(\|A\|^3). \tag{3.1}$$

Proof of (3.1). For diagonal matrices, this can be proved by direct computation. For symmetric matrices A, we can verify it by first diagonalizing A. Finally, for an arbitrary square matrix A, we use the identity

$$\det[I+A] = \sqrt{\det[I+B]},$$

where $B = (A + A^*) + AA^*$ is a symmetric matrix. □

The expansion of g can be written in the matrix form:

$$g(x) = I + 2H|x^1| + L|x^1|^2 - \tfrac{1}{3}C(\tilde{x}, \tilde{x}) + 2\nabla_{\tilde{x}}H|x^1| + O(|x|^3), \tag{3.2}$$

where H, L, $C(\tilde{x}, \tilde{x})$ and $\nabla_{\tilde{x}}H$ are matrices whose components are $H = \{H_{ij}\} =$ the second fundamental form matrix,

$$L = \{-R_{1i1j} + (H^2)_{ij}\}, \quad C(\tilde{x}, \tilde{x}) = \{R^{\partial\Omega}_{ikjl}x^k x^l\}_{2\le i,j\le n},$$

$$\nabla_{\tilde{x}}H = \{\nabla_k H_{ij} x^k\}.$$

Using (3.1) and (3.2), we see that the Taylor expansion of $\det g(x)$ is

$$\begin{aligned}\det g(x) = 1 &+ 2\operatorname{tr} H|x^1| + [2(\operatorname{tr} H)^2 - \operatorname{tr}(H^2) - \operatorname{Ric}(n)]|x^1|^2 \\ &- \tfrac{1}{3}\operatorname{tr} C(\tilde{x}, \tilde{x}) + 2\operatorname{tr} \nabla_{\tilde{x}}H|x^1| + O(|x|^3),\end{aligned}$$

where by definition $\operatorname{Ric}(n) = \sum_{i=2}^n R_{1i1i}$. Hence we have

$$\begin{aligned}J(x) = 1 &+ \operatorname{tr} H|x^1| + \tfrac{1}{2}[(\operatorname{tr} H)^2 - \operatorname{tr} H^2 - \operatorname{Ric}(n)]|x^1|^2 \\ &- \tfrac{1}{6}\operatorname{tr} C(\tilde{x}, \tilde{x}) + \operatorname{tr} \nabla_{\tilde{x}}H|x^1| + O(|x|^3).\end{aligned} \tag{3.3}$$

We also need the Taylor expansion of the inverse matrix of $g(x)$, which will be denoted by $h(x)$. This is done easily with the help of the formula

$$(I+A)^{-1} = I - A + A^2 + O(\|A\|^3).$$

The answer is

$$\begin{aligned}h(x) = I &- 2H|x^1| + [4H^2 - L]|x^1|^2 \\ &+ \tfrac{1}{3}C(\tilde{x}, \tilde{x}) - 2\nabla_{\tilde{x}}H|x^1| + O(|x|^3).\end{aligned} \tag{3.4}$$

As a consequence of (3.4), we see that if none of i, j, k, l is equal to 1, then

$$\partial_i\partial_j h^{kl} = \tfrac{1}{3}\partial_i\partial_j C_{kl}(\tilde{x}, \tilde{x}) = \tfrac{1}{3}(R^{\partial\Omega}_{kilj} + R^{\partial\Omega}_{kjil}). \tag{3.5}$$

The Laplace-Beltrami operator in the local coordinate form is

$$\begin{aligned}\Delta &= \frac{1}{\sqrt{\det g(x)}}\frac{\partial}{\partial x^i}\left[\sqrt{\det g(x)}g^{ij}(x)\frac{\partial}{\partial x^j}\right] \\ &= h^{ij}(x)\frac{\partial}{\partial x^i}\frac{\partial}{\partial x^j} + b^j(x)\frac{\partial}{\partial x^j},\end{aligned} \tag{3.6}$$

where

$$b^j(x) = \frac{1}{J(x)}\frac{\partial}{\partial x^i}[J(x)h^{ij}(x)].$$

Using (3.3), (3.4), and (3.5), we have

(3.7a) $$b^j(\pm 0, \tilde{0}) = \pm \operatorname{tr} H\delta_1^j,$$

(3.7b) $$\nabla_1 b^1(0) = -[\operatorname{Ric}(n) + \operatorname{tr} H^2],$$

(3.7c) $$\partial_1 b^j(0) = \operatorname{tr} \partial_j H - 2\partial_i H_{ij}, \qquad i \neq 1,$$

(3.7d) $$\partial_j b^j(0) = -\frac{2}{3}\sum_{k=2}^{n} R^{\partial\Omega}_{jkjk}, \qquad j \neq 1.$$

4. Localization and the parametrix method

As before Ω is a compact Riemannian manifold with smooth boundary. We consider the double $\tilde{\Omega}$ of Ω defined as follows. Take another copy of Ω and call it Ω^*. The double $\tilde{\Omega}$ is simply the union $\Omega \cup \Omega^*$ with the each corresponding pair of boundary points on Ω and Ω^* identified. Thus symbolically $\tilde{\Omega} = \Omega \cup \Omega^*/\partial\Omega \sim \partial\Omega^*$. Clearly the double $\tilde{\Omega}$ has a natural Riemannian structure which in general has discontinuous derivatives at the boundary of contact of Ω and Ω^*. If x is a point of Ω, we use x^* to denote the point on Ω^* which is symmetric to x. Unless $\partial\Omega$ is totally geodesic (i.e., the second fundamental form vanishes identically) the Laplace-Beltrami operator on $\tilde{\Omega}$ is in general not a smooth operator, but it is easy to see that in local coordinates it is still a second order elliptic operator. The coefficients of its second order derivatives are continuous on $\tilde{\Omega}$ and smooth on Ω and Ω^*. The coefficients of its first order derivatives are smooth on Ω and Ω^* up to the boundary of contact (see Proposition 6 of the last section). We denote the fundamental solution of the heat equation on $\tilde{\Omega}$ by $q(t, x, y)$. Now the fundamental solutions for the heat equation on Ω with the Dirichlet condition or the Neumann condition are, respectively,

(4.1a) $$p_D(t, x, y) = q(t, x, y) - q(t, x^*, y),$$

(4.1b) $$p_N(t, x, y) = q(t, x, y) + q(t, x^*, y).$$

Therefore we have

(4.2) $$\int_\Omega p_N(t, x, x)\,dx = \int_\Omega q(t, x, x)\,dx + \int_\Omega q(t, x^*, x)\,dx.$$

We now divide Ω into two parts. If ε is sufficiently small, then for every point $x \in \Omega$ such that $d(x, \partial\Omega) \le \varepsilon$, there is unique point $z \in \partial\Omega$ such that $d(x, z) = d(x, \partial\Omega)$. It follows that for sufficiently small ε, the set $\Omega_\varepsilon = \{x \in \Omega : d(x, \partial\Omega) \le \varepsilon\}$ can be parametrized by $(x^1, z) \in (0, \varepsilon) \times \partial\Omega$, where $x^1 = d(x, \partial\Omega)$. We fix such an ε and a collar Ω_ε of width ε of the boundary.

There exists a constant $\delta > 0$, depending on ε, such that

(4.3) $$\forall t \le t_0, \qquad \int_{\Omega\setminus\Omega_\varepsilon} q(t, x^*, x)\,dx \le e^{-\delta/t}.$$

This follows easily from (4.12). On the other hand, by [MS, p. 50] we have

$$(4.4)\qquad (4\pi t)^{n/2}q(t, x, x) = 1 + \frac{t}{6}K(x) + O(t^2)$$

uniformly on $\Omega\backslash\Omega_\varepsilon$. Hence from (4.2)–(4.4) we see that

$$(4.5)\qquad (4\pi t)^{n/2}\Theta_N(t) = |\Omega\backslash\Omega_\varepsilon| + \frac{t}{6}\int_{\Omega\backslash\Omega_\varepsilon} K(x)\,dx + I_1(t) + I_2(t) + O(t^2),$$

where

$$I_1(t) = \int_{\Omega_\varepsilon} q(t, x, x)\,dx \quad\text{and}\quad I_2(t) = \int_{\Omega_\varepsilon} q(t, x^*, x)\,dx.$$

We note that the boundary collar Ω_ε is parametrized by $x = (x^1, z)$ with $x^1 = d(x, \partial\Omega)$ and $z \in \partial\Omega$. The volume element dx can be written as $\beta(x)dx^1\sigma(dz)$, where $\sigma(dz)$ is the volume element of the boundary. We can therefore write

$$(4.6)\qquad I_i(t) = \int_U I_i(t, z)\sigma(dz), \qquad i = 1, 2,$$

where

$$(4.7)\qquad \begin{aligned} I_1(t, z) &= \int_0^\varepsilon q(t, x, x)\beta(x)\,dx^1, \\ I_2(t, z) &= \int_0^\varepsilon q(t, x^*, x)\beta(x)\,dx^1. \end{aligned}$$

We will use the parametrix method to write the heat kernel $q(t, x, y)$ as a convergent series and take the first three terms to compute the integrals in (4.7). From the above formula for $I_i(t, z)$, we see that it is enough to construct the heat kernel in a neighborhood of a fixed point $z \in \partial\Omega$. From now on we fix a point $z = O$ on the boundary $\partial\Omega$ and choose the local coordinates in a neighborhood of O as in §3.

The parametrix method works as follows. First of all, since we are only concerned with the heat kernel in a neighborhood of O, by the localization principle, we may modify the metric outside a neighborhood of O as we wish without affecting the asymptotic expansions of $I_i(t, O)$, $i = 1, 2$. This observation allows us to assume, for the purpose of computing the asymptotic expansions, that Ω is the Euclidean half-space R^n_+ $\{x = (x^1, \tilde{x}): x^1 > 0\}$ and the metric matrix g_{ij} is the identity matrix outside some neighborhood of the origin O. We may also assume that $x^1 = d(x, \partial\Omega)(d(\cdot, \cdot)$ is the Riemannian metric), the double $\tilde{\Omega} = R^n$, and that the symmetric reflection is simply $x^* = (-x^1, \tilde{x})$. Under these assumptions the metric matrix in $\Omega^* = \{x = (x^1, \tilde{x}): x^1 < 0\}$ is defined by $g(x^1, \tilde{x}) = g(-x^1, \tilde{x})$.

Now the heat kernel can be expressed as a convergent series:

$$(4.8)\qquad q(t, x, y) = \sum_{m=0}^{\infty} q_m(t, x, y).$$

The functions $q_m(t, x, y)$ are defined recursively as follows:

$$(4.9)\qquad q_0(t, x, y) = \left(\frac{1}{4\pi t}\right)^{n/2} e^{-(y-x)^T g(y)(y-x)/4t},$$

$$q_m(t, x, y) = \int_0^t ds \int_{R^n} q_{m-1}(t-s, x, z) f(s, z, y)\, dz, \tag{4.10}$$

where

$$\begin{aligned} f(s, z, y) &= \left[\Delta_z - g^{ij}(y)\frac{\partial^2}{\partial z^i \partial z^j}\right] q_0(s, z, y) J(z) \\ &= \left[(h^{ij}(z) - h^{ij}(y))\frac{\partial^2}{\partial z^i \partial z^j} + b^j(z)\frac{\partial}{\partial z^j}\right] q_0(s, z, y) J(z). \end{aligned}$$

(See (3.6) for the local expression of Δ.) From now on, if an integral is over R^n, R^n_+, or R^{n-1}, then dz denotes the Euclidean volume element. Note that we have chosen a first approximation $q_0(t, x, y)$ of the heat kernel slightly different from the one in [MS]. It turns out that our choice greatly simplifies the subsequent calculations. (4.8) is obtained by iterating the integral equation

$$q(t, x, y) = q_0(t, x, y) + \int_0 ds \int_{R^n} q(t-s, x, z) f(s, z, y) J(z)\, dz,$$

which can be verified by simple calculation.

It is not difficult to show by induction that $q_m(t, x, y)$ satisfies the following estimate: there exist positive constant t_0, c_0, c_1 such that for all x, y in R^n and $t < t_0$,

$$q_m(t, x, y) \le c_0 c_1^m \Gamma\left(\frac{m+1}{2}\right)^{-1} t^{(m-n)/2} e^{-|x-y|^2/c_1 t}. \tag{4.11}$$

Summing over m, we obtain the basic estimate for the heat kernel

$$q(t, x, y) \le c_2 t^{-n/2} e^{-|x-y|^2/c_1 t}, \tag{4.12}$$

from which (2.3) and (4.3) follow. (4.11) implies

$$t^{n/2} \sum_{m=3}^{\infty} \int_{\Omega_\varepsilon} \{|q_m(t, x, x)| + |q_m(t, x^*, x)|\}\, dx \le c_3 \varepsilon t^{3/2}.$$

Since ε can be chosen arbitrarily small, and we know beforehand that $\Theta_N(t)$ and $\Theta_D(t)$ have asymptotic expansions of the form (1.1) in powers of $t^{1/2}$, an error term of the order $t^{3/2}\varepsilon$ will not affect the computation of the coefficient a_3 of the power $t^{3/2}$.

Now we have from (4.7)

$$I_1(t, z) = \sum_{i=0}^{2} J_i(t) + O(t^{3/2}\varepsilon), \tag{4.13a}$$

$$I_2(t, z) = \sum_{i=0}^{2} K_i(t) + O(t^{3/2}\varepsilon), \tag{4.13b}$$

where

$$J_i(t) = \int_0^\varepsilon q_i(t, x, x) J(x)\, dx^1, \quad K_i(t) = \int_0^\varepsilon q_i(t, x^*, x) J(x)\, dx^1. \tag{4.14}$$

Note that $z = O$ is fixed (the origin of our local coordinates) and $x = (x^1, \tilde{0})$. Also note that in the local coordinates we are using, $\beta(x) = J(x)$.

5. Asymptotic calculations

(a) *Calculation of* $J_0(t)$. We see from (4.9) of the last section that

$$q_0(t, x, x) = \left(\frac{1}{4\pi t}\right)^{n/2}.$$

Therefore we obtain

$$(4\pi t)^{n/2} J_0(t) = (4\pi t)^{n/2} \int_0^\varepsilon q_0(t, x, x) J(x)\, dx^1 = \int_0^\varepsilon J(x)\, dx^1. \tag{5.1}$$

(b) *Calculation of* $K_0(t)$. In the local coordinates we are using, $x^* = (-x^1, \tilde{0})$. Also note that in our coordinates, the metric matrix has a special form, i.e., $g_{1j}(x) = \delta_{1j}$ (Proposition 6). Hence

$$q_0(t, x^*, x) = \left(\frac{1}{4\pi t}\right)^{n/2} e^{-|x^1|^2/t}.$$

Hence

$$(4\pi t)^{n/2} K_0(t) = \int_0^\varepsilon e^{-|x^1|^2/t} J(x)\, dx^1.$$

We now use the asymptotic expansion of $J(x^1, \tilde{0})$ computed in (3.3),

$$J(x^1, \tilde{0}) = 1 + \operatorname{tr} H|x^1| + \tfrac{1}{2}[(\operatorname{tr} H)^2 - \operatorname{tr} H^2 - \operatorname{Ric}(n)]|x^1|^2 + O(|x^1|^3).$$

Therefore, $(4\pi t)^{n/2} K_0(t)$ is equal to

$$\int_0^\varepsilon e^{-|x^1|^2/t} \left\{1 + \operatorname{tr} H x^1 + \frac{1}{2}[(\operatorname{tr} H)^2 - \operatorname{tr} H^2 - \operatorname{Ric}(n)]|x^1|^2 + O(|x^1|^3)\right\} dx^1.$$

After calculating the integrals, we have

$$\begin{aligned}(4\pi t)^{n/2} K_0(t) &= \tfrac{1}{2}\sqrt{\pi t} + \tfrac{1}{2} t \operatorname{tr} H \\ &\quad + \tfrac{1}{8}\sqrt{\pi} t^{3/2}[(\operatorname{tr} H)^2 - \operatorname{tr} H^2 - \operatorname{Ric}(n)] + O(t^2).\end{aligned} \tag{5.2}$$

(c) *Calculation of* $J_1(t)$. We have

$$f(s, y, x) = M(s, x, y) q_0(s, x, y)$$

where

$$\begin{aligned} M(s, x, y; t) &= L(s, x, y) J(y), \\ L(s, x, y) &= \frac{1}{4s^2}(y - x)^T g(x)[h(y) - h(x)] g(x)(y - x) \\ &\quad - \frac{1}{2s}\operatorname{tr}[h(y) - h(x)] g(x) - \frac{1}{2s} b(y)^T g(x)(y - x). \end{aligned} \tag{5.3}$$

Hence

$$J_1(t) = \int_0^\varepsilon J(x)\, dx^1 \int_0^t [4\pi(t - s) 4\pi s]^{-n/2} ds \int_{R^n} e^{-N(s, x, y; t)} M(s, x, y; t)\, dy$$

with

$$N(s, x, y; t) = \frac{(y - x)^T g(y)(y - x)}{4(t - s)} + \frac{(x - y)^T g(x)(x - y)}{4s}.$$

We need to expand $N(s, x, y; t)$ and $M(s, x, y; t)$. We have to be careful because derivatives of $J(y)$, $g(y)$, $h(y)$ and the function $b(y)$ itself have jumps across the hyperplane $y^1 = 0$. For the sake of convenience, we introduce the notation $\hat{y} = (|y^1|, \tilde{y})$. In addition, for a vector $a = (a^1, \dots, a^n)$, we use the notation $\nabla_a h = a^i \partial_i h$, summing from 1 to n. Now since $h(y) = h(\hat{y})$, we have

$$\begin{aligned} h(y) - h(x) &= h(\hat{y}) - h(x) \\ &= \nabla_{\hat{y}-x} h(x) + \tfrac{1}{2} \nabla^2_{\hat{y}-x, \hat{y}-x} h(x) + O(|\hat{y} - x|^3) \\ &= \nabla_{y-x} h(x) + \tfrac{1}{2} \nabla^2_{y-x, y-x} h(x) + \nabla_{\hat{y}-y} h(x) \\ &\quad + \nabla^2_{\hat{y}-y, y-x} h(x) + \tfrac{1}{2} \nabla^2_{\hat{y}-y, \hat{y}-y} h(x) + O(|\hat{y} - x|^3). \end{aligned}$$

Clearly $\hat{y} - y = (\hat{y}^1 - y^1, \tilde{0})$. Using (3.4), we have

$$\begin{aligned} &\nabla_{\hat{y}-y} h(x) + \nabla^2_{\hat{y}-y, y-x} h(x) + \tfrac{1}{2} \nabla^2_{\hat{y}-y, \hat{y}-y} h(x) \\ &\quad = -2(\hat{y}^1 - y^1) H + \tfrac{1}{2} \nabla^2_{\hat{y}-y, \hat{y}+y} h \\ &\qquad - O(|\hat{y} - y|\,|x|^2 + |\hat{y} - y|\,|y - x|\,|x| + |\hat{y} - y|^2 |x|). \end{aligned}$$

It follows that

$$\begin{aligned} h(y) - h(x) &= \nabla_{y-x} h(x) + \tfrac{1}{2} \nabla^2_{y-x, y-x} h(x) - 2(\hat{y}^1 - y^1) H \\ &\quad + O(|\hat{y} - x|^3 + |\hat{y} - y|\,|x|^2 + |\hat{y} - y|\,|y - x|\,|x| + |\hat{y} - y|^2 |x|). \end{aligned}$$

The following elementary inequalities will be used repeatedly below to simplify error terms:

$$|\hat{y} - x| \le |y - x|, \quad |\hat{y} - y| \le |\hat{y} - x| + |y - x| \le 2|y - x|, \quad |y| \le |y - x| + |x|.$$

In order to record various error terms in a more compact form, we adopt the following convention.

Convention A. *If a monomial in time and length has the dimension length^a time^b (b may be negative), then we say that this monomial has the order $a + 2b$. An error term is said to be of the form O_k if it is bounded by a sum of monomials of order k whose length factors are bounded by powers of $|x - y|$. An error term is said to have the form O_k^y if it is of the form O_k and it vanishes when $y^1 \ge 0$.*

For example, an error term of the form $O(|x - y|^3)$ is of the form O_3. An error term $O(|x - y|/s)$ is of the form O_{-1}, an error term of the form $O(|x - y|^2 |x|)$ is of the form $|x| O_2$. An error term of the form $O(|\hat{y} - y|^2 |x|)$ has the form $|x| O_2^y$ since it vanishes when $y^1 \ge 0$ and $|\hat{y} - y|^2 |x| \le 4|x - y|^2 |x|$.

Using Convention A, we can write

$$\begin{aligned} h(y) - h(x) &= \nabla_{y-x} h(x) + \tfrac{1}{2} \nabla^2_{y-x, y-x} h(x) \\ &\quad - 2(\hat{y}^1 - y^1) H + O_3 + |x| O_2^y + |x|^2 O_1^y. \end{aligned}$$

Similarly, we have

$$\begin{aligned} g(y) &= g(x) + \nabla_{y-x} g(x) + 2(\hat{y}^1 - y^1) H + O_2 + |x| O_1^y, \\ J(y) &= J(x) + \nabla_{y-x} J(x) + (\hat{y}^1 - y^1) \operatorname{tr} H + O_2 + |x| O_1^y. \end{aligned}$$

The expansion of $b(y)$ is a little more complicated. Noting that $h^{1j} = \delta^{1j}$ and $\hat{y} = (|y^1|, \tilde{y})$ we have

$$\begin{aligned} b^j(y) &= \frac{1}{J(\hat{y})}\frac{\partial}{\partial y^i}[J(\hat{y})h^{ij}(\hat{y})] \\ &= b^j(\hat{y}) + [\operatorname{sgn} y^1 - 1]\delta^{1j}\partial_1[J](\hat{y}) \\ &= b^j(x) + \nabla_{y-x}b^j(x) + (\hat{y}^1 - y^1)\partial_1 b^j \\ &\quad + [\operatorname{sgn} y^1 - 1]\delta^{1j}[\partial_1 J + \nabla_{\hat{y}}\partial_1 J] + O_2 + |x|^2 O_0^y. \end{aligned}$$

Using (3.3), (3.7b), and (3.7c) we have

$$\begin{aligned} &(\hat{y}^1 - y^1)\partial_1 b^j + [\operatorname{sgn} y^1 - 1]\delta_{1j}\nabla_{\hat{y}}\partial_1 J \\ &\quad = -(\hat{y}^1 - y^1)\delta^{1j}(\operatorname{tr} H)^2 + (\hat{y}^1 - y^1)[\operatorname{tr} \partial_j H - 2\partial_i H_{ij}] \\ &\quad\quad + [\operatorname{sgn} y^1 - 1]\delta^{1j}\operatorname{tr} \nabla_{\hat{y}} H. \end{aligned}$$

It follows that

$$\begin{aligned} b^j(y) &= b^j(x) + \nabla_{y-x}b^j(x) + [\operatorname{sgn} y^1 - 1]\delta^{1j}[\operatorname{tr} H + \operatorname{tr} \nabla_{\hat{y}} H] \\ &\quad - (\hat{y}^1 - y^1)\delta^{1j}(\operatorname{tr} H)^2 + (\hat{y}^1 - y^1)[\operatorname{tr} \partial_j H - 2\partial_i H_{ij}] \\ &\quad + O_2 + |x|^2 O_0^y. \end{aligned} \tag{5.4}$$

We now discuss the expansions of $N(s, x, y; t)$ and $M(s, x, y; t)$. Let us first discuss $N(s, x, y; t)$. Using the expansion for $g(y)$ above, we have

$$\begin{aligned} N(s, x, y; t) &= N_0(s, x, y; t) + \frac{1}{4(t-s)}(y-x)^T\nabla_{y-x}g(x)(y-x) \\ &\quad + \frac{1}{2(t-s)}(\hat{y}^1 - y^1)\tilde{y}H^T\tilde{y} + O_2 + |x|O_1^y \end{aligned}$$

where

$$N_0(s, x, y; t) = \frac{1}{4r}(y-x)^T g(x)(y-x), \qquad \left[r = \frac{s(t-s)}{t}\right].$$

As will be explained below, we can always restrict the integration in y variables to the region $|y-x| \le (t-s)^{2/5}$. If $|y-x| \le (t-s)^{2/5}$, we have

$$\begin{aligned} e^{-N(s,x,y;t)} &= e^{-N_0(s,x,y;t)}\left[1 + \frac{1}{4(t-s)}(y-x)^T\nabla_{y-x}g(x)(y-x)\right] \\ &\quad + e^{-N_0(s,x,y;t)}\frac{1}{2(t-s)}(\hat{y}^1 - y^1)\tilde{y}^T H\tilde{y} \\ &\quad + e^{-N_0(s,x,y;t)}[O_2 + |x|O_1^y]. \end{aligned} \tag{5.5}$$

Now using the elementary relation

$$e^{-a} = e^{-b} + e^{-\min\{a,b\}}O(|a-b|), \qquad a \ge 0,\ b \ge 0,$$

and the inequality

$$|x|^k e^{-c|x|^2} \le c_1 e^{-c_2|x|^2}, \qquad k \ge 0,$$

we have

$$e^{-N_0(s,x,y;t)} = e^{-N_{00}(s,x,y;t)} + e^{-cN_{00}(s,x,y;t)}O(|x|) \tag{5.6}$$

where

$$N_{00}(s, x, y; t) = \frac{1}{4r}|y - x|^2.$$

We replace the exponential factor e^{-N_0} in the second and the third term on the right-hand side of (5.5) by the right-hand side of (5.6) and obtain for $|x-y| \le (t-s)^{2/5}$

$$\begin{aligned} e^{-N(s,x,y;t)} &= e^{-N_0(s,x,y;t)}\left[1 + \frac{1}{4(t-s)}(y-x)^T\nabla_{y-x}g(x)(y-x)\right] \\ &\quad + e^{-N_{00}(s,x,y;t)}\frac{1}{2(t-s)}(\hat{y}^1 - y^1)\tilde{y}^T H\tilde{y} \\ &\quad + e^{-cN_{00}(s,x,y;t)}[O_2 + |x|O_1^y]. \end{aligned} \tag{5.7a}$$

To simplify notation, we sometimes use the abbreviated symbol N for $N(s,x,y;t)$, N_0 for $N_0(s,x,y;t)$, etc.

Another kind of expansion of e^{-N} is as follows. We have

$$N = N_{00} + \frac{1}{4}\left[\frac{\hat{y}^1}{(t-s)} + \frac{x}{s}\right]\tilde{y}^T H\tilde{y} + O_2 + |x|^2 O_0.$$

As will be explained below, we can restrict the integration to the region

$$|y-x| \le r^{2/5} \le \min\{(t-s)^{2/5}, s^{2/5}\}, \qquad |x| \le r^{2/5} \le \min\{(t-s)^{2/5}, s^{2/5}\}.$$

If these conditions are satisfied, we have

$$\begin{aligned} e^{-N} &= e^{-N_{00}} + e^{-N_{00}}\frac{1}{4}\left[\frac{\hat{y}^1}{(t-s)} + \frac{x^1}{s}\right]\tilde{y}^T H\tilde{y} \\ &\quad + e_{00}^{-cN_{00}}[O_2 + |x|O_1 + |x|^2 O_0]. \end{aligned} \tag{5.7b}$$

We call (5.7a) the mixed expansion (at x at O), and (5.7b) the expansion at O.

For the expansions of $J(y)$ we have the mixed expansion

$$J(y) = J_0(x, y) + (\hat{y}^1 - y^1)\operatorname{tr} H + O_2 + |x|O_1^y, \tag{5.8a}$$

where

$$J_0(x, y) = J(x) + \nabla_{y-x}J(x),$$

and the expansion at O,

$$J(y) = J(\hat{y}) = 1 + \hat{y}^1\operatorname{tr} H + O_2 + |x|^2 O_1^y. \tag{5.8b}$$

We also need two expansions of $L(s, x, y)$. The mixed expansion of $L(s, x, y)$ is

$$\begin{aligned} L(s, x, y; t) &= L_0(s, x, y) - \frac{1}{2s^2}(\hat{y}^1 - y^1)\tilde{y}^T[H + \nabla_{\tilde{y}}H]\tilde{y} \\ &\quad + \frac{1}{s^2}x^1(y^1 - x^1)\tilde{y}^T H^2\tilde{y} + \frac{1}{s}(\hat{y}^1 - y^1)\operatorname{tr}[H + \nabla_{\tilde{y}}H] \\ &\quad + \frac{1}{s}(\hat{y}^1 - y^1)x^1\operatorname{tr} H^2 - \frac{1}{2s}[\operatorname{sgn} y^1 - 1](y^1 - x^1)[\operatorname{tr} H + \operatorname{tr}\nabla_{\tilde{y}}H] \\ &\quad + \frac{1}{2s}(\hat{y}^1 - y^1)(y^1 - x^1)\operatorname{tr} H^2 - \frac{1}{2s}(\hat{y}^1 - y^1)[\operatorname{tr}\nabla_{\tilde{y}}H - 2y^j\partial_i H^{ij}] \\ &\quad + O_1 + |x|O_0^y + |x|^2 O_{-1}^y, \end{aligned} \tag{5.9a}$$

where
(5.10)

$$L_0(s, x, y) = \frac{1}{4s^2}(y-x)^T g(x)\left[\nabla_{y-x}h(x) + \frac{1}{2}\nabla^2_{y-x,y-x}h(x)\right] g(x)(y-x)$$
$$- \frac{1}{2s}\mathrm{tr}\left[\nabla_{y-x}h(x) + \frac{1}{2}\nabla_{y-x,y-x}h(x)\right] g(x)$$
$$- \frac{1}{2s}[b(x) + \nabla_{y-x}b(x)]^T g(x)(y-x).$$

The expansion of L at O is

(5.9b) $$L(s, x, y) = L_{00}(s, x, y) + O_0 + |x|O_{-1},$$

where

$$L_{00}(s, x, y) = -\frac{1}{2s^2}(y^1 - x^1)\tilde{y}^T H\tilde{y} + \frac{1}{2}(y^1 - x^1)\mathrm{tr}\, H$$
$$- \frac{1}{2s}(y^1 - x^1)\mathrm{sgn}\, y^1 \mathrm{tr}\, H.$$

We now state another convention.

Convention B. *We will use F_k to denote a general polynomial of order k (in the sense of Convention A) in the variables $\hat{y}^1$, y^1, x^1, s^{-1}, and $(t-s)^{-1}$. A general polynomial of the form F_k which vanishes on $y^1 \geq 0$ will be denoted by F_k^y. Furthermore, we will use G to denote a polynomial of the following form:*

$$G = F_{-2}\tilde{y}^T H^2\tilde{y} + F_{-4}(\tilde{y}^T H\tilde{y})^2 + F_{-2}\tilde{y}^T H\tilde{y}\mathrm{tr}\, H + F_0(\mathrm{tr}\, H)^2$$
$$+ F_0\mathrm{tr}\, H^2 + F_{-3}\tilde{y}^T\nabla_{\tilde{y}}H\tilde{y} + F_{-1}\mathrm{tr}\, \nabla_{\tilde{y}}H + F_{-1}y^j\partial_i H_{ij}.$$

G^y is a general polynomial of the above form which vanishes when $y^1 \geq 0$.

Using Convention B, (5.9a) can be written as

(5.9a) $$L(s, x, y; t) = L_0(s, x, y) + L^y_{000}(s, x, y) + G^y + O_1 + |x|O^y_0 + |x|^2 O^y_{-1},$$

where

$$L^y_{000}(s, x, y) = -\frac{1}{2s^2}(\hat{y}^1 - y^1)\tilde{y}^T H\tilde{y} - \frac{1}{s}\chi_{(\infty,0]}(y^1)(x^1 + y^1)\mathrm{tr}\, H.$$

Note that L^y_{000} vanishes when $y^1 \geq 0$. To get the extension of M, we use

$$M = LJ = L_0J_0 + L(J - J_0) + (L - L_0)J - (L - L_0)(J - J_0).$$

Using the expansions (5.8a) and (5.9b) in the second term, the expansions (5.8b) and (5.9a) in the third term, and (5.8b) and (5.9b) in the fourth term, we obtain

(5.11a) $$M(s, x, y) = M_0(s, x, y) + L^y_{000}(s, x, y) + G^y + O_1 + |x|O^y_0 + |x|^2 O^y_{-1},$$

where

$$M_0(s, x, y) = L_0(s, x, y)J_0(x, y).$$

The expansion of M at O can be computed from (5.8b) and (5.9b). We only need terms of order -1. Hence

(5.11b) $$M(s, x, y) = L_{00}(s, x, y) + O_0 + |x|O_{-1}.$$

Using Convention B, we rewrite (5.7a) and (5.7b). If $|x-y| \leq r^{2/5}$, then

$$e^{-N} = e^{-N_0}S_0 + e^{-N_{00}}F_{-1}^y \tilde{y}^T H\tilde{y} + e^{-cN_{00}}[O_2 + |x|O_1^y] \tag{5.12a}$$

and if $|x-y| \leq r^{2/5}$, $|x| \leq r^{2/5}$, then

$$e^{-N} = e^{-N_{00}}[1 + F_{-1}\tilde{y}^T H\tilde{y}] + e^{-cN_{00}}[O_2 + |x|O_1 + |x|^2 O_0] \tag{5.12b}$$

where

$$S_0 = S_0(s, x, y; t) = 1 + \frac{1}{4(t-s)}(y-x)^T \nabla_{y-x} g(x)(y-x).$$

Now

$$\begin{aligned} e^{-N}M = {} & e^{-N_0}S_0M_0 + e^{-N}(M - M_0) + (e^{-N} - e^{-N_0}S_0)M \\ & - (e^{-N} - e^{-N_0}S_0)(M - M_0). \end{aligned} \tag{5.13}$$

Substituting (5.11) and (5.12) into the above identity, we obtain

$$\begin{aligned} e^{-N}M = {} & e^{-N_0}S_0M_0 + e^{-N_{00}}L_{000}^y \\ & + e^{-N_{00}}G^y + e^{-cN_{00}}[O_1 + |x|O_0^y + |x|^2 O_{-1}^y]. \end{aligned} \tag{5.14}$$

Since (5.12a) and (5.12b) hold only under the range of x, y, t, s specified for them, we need to justify their use in (5.13). Recall that $r = s(t-s)/t$. Since

$$e^{-N(s,x,y;t)}|M(s, x, y)| \leq \frac{c_1}{\sqrt{s}}e^{-c_2|x-y|^2/r}$$

for some constants c_1, c_2,

$$\int_0^t r^{-n/2}ds \int_{|y-x|\geq r^{2/5}} \frac{1}{\sqrt{s}}e^{-c_2|x-y|^2/r}dy \leq c_3 e^{-c_4 t^{-1/5}},$$

(compare with [MS, p. 57]), we see that the integration of y can be restricted to the region $|y-x| \leq r^{2/5}$. This justifies the use of (5.12a) in (5.13). Next, to justify the use of (5.12b) in, say, the second term of (5.13), we first note that from (5.11a), $M - M_0$ is the sum of $L_{000}^y + G^y$, which vanishes on $y^1 \geq 0$, and the error terms $O_1 + |x|O_0^y + |x|^2 O_{-1}^y$. Clearly

$$e^{-N(s,x,y;t)}|L_{000}^y + G^y| \leq \frac{c_1}{\sqrt{s}}e^{-c_2|x-y|^2/r}.$$

After the integration, the error terms $O_1 + |x|O_0^y + |x|^2 O_{-1}^y$ will contribute a term of order $O(t^{3/2}\varepsilon + t^2)$ to the final result (see below). The integration of $L_{000}^y + G^y$ can be restricted to the region $x^1 \leq r^{2/5} \leq r^{2/5}$, because

$$\begin{aligned} & \iint_{\substack{0\leq s\leq t \\ x^1 \geq r^{2/5}}} dx^1 r^{-n/2} ds \int_{R^n} \frac{1}{\sqrt{s}} e^{-c_2|x-y|^2/r}\, dy \\ & \leq c_3 \iint_{\substack{0\leq s\leq t \\ x^1 \geq r^{2/5}}} dx^1 r^{-1/2} ds \int_{x_1}^{\infty} \frac{1}{\sqrt{s}} e^{-c_2|w|^2/r}\, dw \\ & \leq c_3 \int_0^t \frac{1}{\sqrt{sr}} ds \int_{r^{2/5}}^{\infty} e^{-c_2|w|^2/r}(w - s^{2/5})\, dw \\ & \leq c_4 \int_0^t \sqrt{\frac{r}{s}} e^{-c_2 r^{-1/5}}\, ds \\ & \leq c_5 e^{-c_2 t^{-1/5}}. \end{aligned}$$

The other terms in (5.13) can be treated in the same way.

We now return to (5.14). A careful observation reveals that the contribution of the term S_0M_0 is

$$\int_0^t \left[\frac{1}{4\pi r}\right]^{n/2} ds \int_{R^n} e^{-N_0} S_0 M_0 dy = \frac{t}{6} K_1(x) J(x) + O(t^2),$$

for some function $K_1(x)$ whose explicit expression is unimportant. Note that there are no terms of order $\sqrt{t}$ because the terms of order -1 in S_0M_0 are odd functions of $y-x$. The contributions of various other terms in (5.14) are straightforward and the results are as follows: the contribution of L^y_{000} is $\alpha_1 t \operatorname{tr} H$, the contribution of G^y is $\alpha_2 t^{3/2}(\operatorname{tr} H)^2 + \alpha_2 t^{3/2} \operatorname{tr} H^2$, the contribution of $O_1 + |x| O_0^y + |x|^2 O_{-1}^y$ is $O(t^{3/2}\varepsilon + t^2)$. Therefore we obtain

$$(5.15)\qquad \begin{aligned}(4\pi t)^{n/2} J_1(t) &= \alpha_0 t \operatorname{tr} H + t\int_0^{\varepsilon} K_1(x) J(x)\, dx^1 \\ &\quad + t^{3/2}[\alpha_1(\operatorname{tr} H)^2 + \alpha_2 \operatorname{tr} H^2] + O(t^{3/2}\varepsilon + t^2).\end{aligned}$$

In fact $\alpha_0 = -1/3$. This completes the calculation of $J_1(t)$.

(d) *Computation of* $K_1(t)$. We have

$$(4\pi t)^{n/2} q_1(t, x^*, x) = \int_0^t \left[\frac{1}{4\pi r}\right]^{n/2} ds \int_{R^n} e^{-N^*(s,x,y;t)} M(s, x, y; t)\, dy,$$

where $M = M(s, x, y)$ is the same as before and

$$N^* = N^*(s, x, y; t) = \frac{(y-x^*)^T g(y)(y-x^*)}{4(t-s)} + \frac{(x-y)^T g(x)(x-y)}{4s}.$$

In the present case we only need the expansions of N^* and M at O. We have

$$N^* = N_0^* + \frac{1}{4}\left[\frac{\hat{y}^1}{t-s} + \frac{x^1}{s}\right] \tilde{y}^T H \tilde{y} + O_2 + |x|^2 O_0,$$

where

$$N_0^* = N_0^*(s, x, y; t) = \frac{|y^1 + x^1|^2}{4(t-s)} + \frac{|y^1 - x^1|^2}{4s} + \frac{t}{4s(t-s)}|\tilde{y}|^2.$$

As before the integration can be restricted to the region $|y-x| \le r^{2/5}$, $|x| \le r^{2/5}$. If these conditions are satisfied,

$$e^{-N^*} = e^{-N_0^*}[1 + F_{-1}\tilde{y}^T H \tilde{y}] + e^{-cN_0^*}[O_2 + |x|^2 O_0].$$

The expansion of $M = M(s, x, y; t)$ at O has been computed before in (5.11b). But this time we need the precise zeroth order terms. From (5.11a) and $M_0 = L_0 J_0$, we see that the only zeroth order terms of M which are not incorporated in G come from the zeroth order terms of L_0 in (5.10). We have

$$\nabla_{y-x} h(x) + \tfrac{1}{2}\nabla^2_{y-x,y-x} h(x) = \tfrac{1}{2}\nabla_{y-x,y+x} h + O(|x-y|^3).$$

Now

$$\nabla^2_{y-x,y+x} h = \nabla^2_{y,y} h - |x^1|^2 \nabla_{1,1} h,$$

and

$$\nabla_{y,y} h = |y^1|^2 \nabla^2_{1,1} h + 2y^1 y^i \nabla^2_{1,i} h + y^i y^j \nabla^2_{i,j} h,$$

Since we know from (5.11b) that the (-1)th order part of M is L_{00}, we have

$$\begin{aligned} M - L_{00} = {} & \frac{1}{8s^2}|y^1|^2 y^k y^l \nabla_{1,1} h^{kl} + \frac{1}{4s^2} y^1 y^i y^k y^l \nabla^2_{1,i} h^{kl} + \frac{1}{8s^2} y^i y^j y^k y^l \nabla_{i,j} h^{kj} \\ & - \frac{1}{8s^2}|x^1|^2 y^k y^l \nabla^2_{1,1} h^{kl} - \frac{1}{4s}|y^1|^2 \operatorname{tr} \nabla^2_{1,1} h - \frac{1}{2s} y^1 y^i \nabla^2_{1,i} h^{kk} \\ & - \frac{1}{4s} y^i y^j \nabla^2_{i,j} h^{kk} + \frac{1}{4s}|x^1|^2 \operatorname{tr} \nabla^2_{1,1} h - \frac{1}{2s} y^1 (y^1 - x^1) \partial_1 b^1 \\ & - \frac{1}{2s} y^1 y^j \partial_1 b^j - \frac{1}{2s}(y^1 - x^1) y^j \partial_j b^1 - \frac{1}{2s} y^i y^j \partial_i b^j \\ & + G + O_1 + |x| O_0. \end{aligned}$$

We claim that the third term is equal to zero. Indeed, by (3.5), this term is equal to $C_0/24s^2$, where

$$\begin{aligned} C_0 &= \nabla^2_{i,j} h^{kl} y^i y^j y^k y^l = \{R_{kilj} + R_{kjli}\} y^i y^j y^k y^l \\ &= 2R_{kilj} y^i y^j y^k y^l = -2R_{iklj} y^i y^j y^k j^l = -C_0. \end{aligned}$$

Hence $C_0 = 0$. When integrating $\int_{R^n} e^{-N_0^*}(M - L_{00})\, dy$, we may drop the terms in $M - L_{00}$ which are odd functions of $\tilde{y}$ because these terms will contribute nothing to the final result. Thus we have

$$\begin{aligned} & \int_{R^n} e^{-N_0^*(s,x,y;t)} M(s,x,y)\, dy \\ & \quad = \int_{R^n} e^{-N_0^*(s,x,y;t)} M_1(s,x,y)\, dy \\ & \qquad + \int_{R^n} e^{-N^*(s,x,y;t)} L_{00}(s,x,y)\, dy + \int_{R^n} e^{-N^*}[G + O_1 + |x| O_0]\, dx \end{aligned}$$

where

$$\begin{aligned} M_1(s,x,y;t) = {} & \frac{1}{8s^2}[|y^1|^2 - |x^1|^2]|y^k|^2 \nabla^2_{1,1} h^{kk} - \frac{1}{4s}[|y^1|^2 - |x^1|^2] \operatorname{tr} \nabla^2_{1,1} h \\ & - \frac{1}{4s}|y^i|^2 \nabla^2_{i,i} h^{kk} - \frac{1}{2s} y^1 (y^1 - x^1) \partial_1 b^1 - \frac{1}{2s}|y^j|^2 \partial_j b^j. \end{aligned}$$

Using (3.4), (3.5) and (3.7), we have

$$\begin{aligned} & M_1(s,x,y) \\ & \quad = \frac{1}{8s^2}[|y^1|^2 - |x^1|^2]|y^k|^2 (4H^2 - L)_{kk} - \frac{1}{4s}[|y^1|^2 - |x^1|^2] \operatorname{tr}(4H^2 - L) \\ & \qquad + \frac{1}{4s}|y^i|^2 R^{\partial\Omega}_{kiki} + \frac{1}{2s} y^1 (y^1 - x^1)|y^1|^2 (\operatorname{Ric}(n) + \operatorname{tr} H^2) + \frac{1}{3s}|y^j|^2 R^{\partial\Omega}_{jkjk}. \end{aligned}$$

Hence after calculating a few definite integrals, we have

$$\begin{aligned} & t^{-3/2} \cdot \int_0^\varepsilon \int_0^t \left[\frac{1}{4\pi r}\right]^{n/2} \int_{R^n} e^{-N_0} M_1\, dy \\ & \quad = \frac{1}{12} K^{\partial\Omega} + \frac{\sqrt{\pi}}{4} \operatorname{Ric}(n) + c_1 \operatorname{tr} H^2 + O(t^{1/2}). \end{aligned} \tag{5.16}$$

We also have

$$\begin{aligned} & \int_0^\varepsilon dx^1 \int_0^t \left[\frac{1}{4\pi r}\right]^{n/2} ds \int_{R^n} e^{-N_{00}^*(s,x,y;t)} L_{00}(s,x,y)\, dy \\ & \quad = c_1 t^{3/2} \operatorname{tr} H + O(t^2). \end{aligned} \tag{5.17}$$

We have as before

$$\int_0^\varepsilon dx^1 \int_0^t r^{-n/2} ds \int_{R^n} e^{-N_0^*(s,x,y;t)} G(s,x,y)\,dy \\ = t^{3/2}[c_1(\operatorname{tr} H)^2 + c_2 \operatorname{tr} H^2] + O(t^2). \tag{5.18}$$

It now follows from (4.14), (5.9), (5.16)–(5.18) that

$$(4\pi t)^{n/2} K_1(t) = \beta_0 t \operatorname{tr} H + \frac{1}{12} t^{3/2} K^{\partial\Omega} + \frac{\sqrt{\pi}}{4} t^{3/2} \operatorname{Ric}(n) \\ + t^{3/2}[\beta_1 (\operatorname{tr} H)^2 + \beta_2 \operatorname{tr} H^2] + O(t^2). \tag{5.19}$$

In fact, we have $\beta_0 = -1/2$. The computation of $K_1(t)$ is completed.

(e) *Calculation of* $J_2(t)$. We now compute the term $J_2(t)$. We have

(5.20)

$$(4\pi t)^{n/2} q_2(t,x,x) = \int_0^t ds \int_0^{t-s} \left[\frac{1}{(4\pi)^2 p}\right]^{n/2} du \\ \times \int_{R^n} dz \int_{R^n} e^{-K(s,u,x,y,z;t)} M(s,x,z) M(u,z,y)\,dy,$$

where

$$p = \frac{t}{su(t-s-u)},$$

$$K = K(s,u,x,y,z;t) = \frac{(y-x)^T g(y)(y-x)}{4(t-s-u)} \\ + \frac{(z-y)^T g(z)(z-y)}{4\pi u} + \frac{(x-z)^T g(x)(x-z)}{4s}$$

and M is defined as before. Expanding K at x we obtain

$$K = \frac{(y-x)^T g(x)(y-x)}{4(t-s-u)} + \frac{(z-y)^T g(x)(z-y)}{4\pi u} \\ + \frac{(x-z)^T g(x)(x-z)}{4s} + O_1. \tag{5.21}$$

As before, the integrations can be restricted to the region

$$|y-x| \le (t-s-u)^{2/5}, \qquad |z-x| \le u^{2/5}, \qquad |z-y| \le u^{2/5}.$$

If these conditions are satisfied, we have

$$e^{-K} = e^{-K_0} + e^{-cK_{00}} O_1, \quad e^{-K_0} = e^{-K_{00}} + e^{-cK_{00}} O(|x|),$$

where K_0 is the sum of the first three terms of the right side of (5.10) and

$$K_{00}(s,u,x,y,z;t) = \frac{|y-x|^2}{4(t-s-u)} + \frac{|z-y|^2}{4\pi u} + \frac{|x-z|^2}{4s}.$$

For the expansion of $M(s,x,z)$, we only need the terms of order -1. We have

$$M(s,x,z) = M_1(s,x,z) + F_{-3}^z \tilde{z}^T H \tilde{z} + F_{-1}^z \operatorname{tr} H + O_0 + |x| O_{-1}^z, \tag{5.22a}$$

where

$$M_1(s,x,z) = \frac{1}{4s^2}(z-x)^T g(x) \nabla_{z-x} h(x) g(x)(z-x) J(x) \\ - \frac{1}{2s} \operatorname{tr} \nabla_{z-x} h(x) g(x) J(x) - \frac{1}{2s} b(x) g(x)(z-x) J(x).$$

The expansion of $M(s, x, z)$ at O has been calculated in (5.11b), i.e.,

(5.22b) $$M(s, x, z) = L_{00}(s, x, z) + O_0 + |x|O_{-1}.$$

We now compute the expansion of $M(u, z, y)$. First of all, we have

$$M(u, z, y) = \frac{1}{4u^2}(y-z)^T g(z)[h(\hat{y}) - h(\hat{z})]g(z)(y-z)J(z) - \frac{1}{2u}\text{tr}[h(\hat{y}) - h(\hat{z})]g(z)J(z) - \frac{1}{2u}b(z)^T g(z)(y-z)J(z).$$

Now we have

$$h(\hat{y}) - h(\hat{z}) = \nabla_{y-z}h(x) + [(\hat{y}^1 - y^1) - (\hat{z}^1 - z^1)]\text{tr } H + O_2 + |x|[O_1^y + O_1^z],$$

$$J(z) = 1 + O_1, \quad b^j(z) = b^j(x) - 2\delta 1j\chi_{(-\infty,0]}(z^1)\text{tr } H + O_1 + |x|O_1^z.$$

Hence

(5.23a) $$\begin{aligned} M(u, z, y) = {} & M_2(u, y-z, x) + F_{-3}^y(\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) \\ & + F_{-3}^z(\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) + F_{-1}^y \text{tr } H + F_{-1}^z \text{tr } H \\ & + O_0 + |x|[O_1^y + O_1^z], \end{aligned}$$

where

$$M_2(u, z-y, x) = \frac{1}{4s^2}(y-z)^T g(x)\nabla_{y-z}h(x)g(x)(y-x)J(x) - \frac{1}{2s}\text{tr } \nabla_{y-z}h(x)g(x)J(x) - \frac{1}{2s}b(x)^T g(x)(y-z)J(x).$$

Also we have

(5.23b) $$\begin{aligned} M(u, z, y) = {} & F_{-3}(\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) + F_{-1}\text{tr } H \\ & + O_0 + |x|[O_{-1}^y + O_{-1}^z]. \end{aligned}$$

Thus from (5.22) and (5.23)

$$\begin{aligned} M(s, x, z)M(u, z, y) = {} & M_1(s, x, z)M_2(u, z, y) + P^{y,z} \\ & + O_{-1} + |x|[O_{-2}^y + O_{-2}^z] \end{aligned}$$

where $P^{y,z}$ stands for a general term of the form

$$\begin{aligned} P^{y,z} = {} & F_{-6}^y \tilde{y}^T H\tilde{y} \cdot (\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) + F_{-6}^z \tilde{z}^T H\tilde{z} \cdot (\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) \\ & + F_{-4}^y \tilde{y}^T H\tilde{y}\text{tr } H + F_{-4}^z \tilde{z}^T H\tilde{z} + F_{-3}^y F_{-3}^z \tilde{y}^T H\tilde{y} \cdot (\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) \\ & + F_{-3}^y F_{-1}^z \tilde{y}^T H\tilde{y}\text{tr } H + F_{-4}^y(\tilde{y} - \tilde{z})^T H(\tilde{y} - \tilde{z}) + F_{-2}^y(\text{tr } H)^2 + F_{-2}^z(\text{tr } H)^2. \end{aligned}$$

The integrand of the y, z integration in (5.20) is then equal to

(5.24) $$\begin{aligned} e^{-K}M(s, x, z)M(u, z, y) = {} & e^{-K_0}M_1(s, x, z)M_2(u, z, y) + e^{-K_{00}}P^{y,z} \\ & + e^{-cK_{00}}[O_{-1} + |x|O_{-2}^y + |x|O_{-2}^z]. \end{aligned}$$

Recall that

(5.25) $$J_2(t) = \int_0^\varepsilon q_2(t, x, x)\,dx^1.$$

Substitute (5.22) into (5.20), and then substitute (5.20) into (5.25). The contribution of M_1M_2 to $J_2(t)$ is

$$\int_0^\varepsilon dx^1 \int_0^t ds \int_0^{t-s} du \left[\frac{1}{(4\pi)^2 p}\right]^{n/2} \int_{R^n} dy \int_{R^n} e^{-K_0} M_1 M_2 dz \\ = \frac{t}{6} K_2(x) J(x) + O(t^2).$$

The contributions of other terms in (5.24) to $J_2(t)$ are as follows: the contribution of $e^{-K_{00}} P^{y,z}$ is $t^{3/2}[\gamma_1(\text{tr } H)^2 + \gamma_2 \text{tr } H^2] + O(t^2)$, the contribution of $e^{-cK_{00}} O_{-1}$ is $O(t^{3/2}\varepsilon)$, the contribution of $e^{-cK_{00}}|x|\{O_{-2}^y, O_{-2}^z\}$ is $O(t^2)$. Summing up, we conclude that

$$(5.26) \qquad (4\pi t)^{n/2} J_2(t) = \frac{t}{6}\int_0^\varepsilon K_2(x) J(x) dx^1 \\ + t^{3/2}[\gamma_1(\text{tr } H)^2 + \gamma_2 \text{tr } H^2] + O(t^{3/2}\varepsilon + t^2).$$

(f) *Calculation of* $K_2(t)$. The computation of $K_2(t)$ is similar to that of $J_2(t)$. The expression for $q_2(t, x^*, x)$ is the same for that of $q_2(t, x, x)$ except that the function K there should be replaced by

$$K^*(s, u, x, y, z; t) = \frac{(y-x^*)^T g(y)(y-x^*)}{4(t-s-u)} \\ + \frac{(z-y)^T g(z)(z-y)}{4\pi u} + \frac{(x-z)^T g(x)(x-z)}{4s}.$$

We only need to expand the integrand at O up to the terms of order -2. We have

$$M(s, x, z) M(u, z, y) = P$$

where P is defined as $P^{y,z}$ but with superscripts y, z removed. We can replace K^* by K_0^*, which is obtained from K^* by setting $g(x)$, $g(y)$, and $g(z)$ in the definition of K^* equal to the identity matrix. The result is

$$(5.27) \qquad K_2(t) = t^{3/2}[\delta_1(\text{tr } H)^2 + \delta_2 \text{tr } H^2] + O(t^2).$$

We have now completed the computations of $J_i(t)$, $K_i(t)$, $i = 0, 1, 2$. Combining the results (4.5)–(4.7), (4.13), (5.1), (5.2), (5.15), (5.19), (5.26), and (5.27), we draw the following conclusion about the coefficient a_3 in the asymptotic expansion of $\Theta_N(t)$ and $\Theta_D(t)$.

Lemma 7. (i) *The coefficient* a_3 *in the expansion of the function* $\Theta_N(t)$ *has the following form*

$$a_3 = \int_{\partial\Omega} a_3(z)\sigma(dz)$$

where

$$(5.28) \qquad a_3(z) = AK^{\partial\Omega}(z) + B\text{Ric}(n) + C(\text{tr } H(z))^2 + D\text{tr } H(z)^2$$

with $A = \sqrt{\pi}/12$ *and* $B = \sqrt{\pi}/8$ *and some constants* C, D;

(ii) *The coefficients* a_3 *in the expansion of the function* $\Theta_D(t)$ *has the following form*

$$a_3 = \int_{\partial\Omega} a_3(z)\sigma(dz)$$

where

$$a_3(z) = AK^{\partial\Omega}(z) + B\mathrm{Ric}(n) + C(\mathrm{tr}\, H(z))^2 + D\mathrm{tr}\, H(z)^2 \tag{5.29}$$

with $A = -\sqrt{\pi}/12$ *and* $B = -\sqrt{\pi}/8$ *and with some constants* C, D. □

We end this section with the

(g) *Proof of Proposition* 4. For any $z \in \partial\Omega$ we have

$$p_N(t, z, z) = 2q(t, z, z) = 2q_0(t, z, z) + 2q_1(t, z, z) + O(t^{(2-n)/2}). \tag{5.30}$$

By definition

$$(4\pi t)^{n/2} q_1(t, z, z) = \int_0^t [4\pi r]^{-n/2} \int_{R^n} e^{-N(s, z, y; t)} M(s, z, y)\, dy. \tag{5.31}$$

The expansion of the integrand at $z = O$,

$$e^{-N} M = e^{-N_{00}} \frac{1}{2}\left[-\frac{y^1}{s^2}\tilde{y}^T H \tilde{y} + \frac{y^1}{s}\mathrm{tr}\, H\right] + e^{-cN_{00}} O_0.$$

Hence after some explicit calculations, we obtain

$$(4\pi t)^{n/2} q_1(t, z, z) = -\tfrac{1}{4}\sqrt{\pi t}\,\mathrm{tr}\, H + O(t). \tag{5.32}$$

Now from (5.30)–(5.32) we have

$$(4\pi t)^{n/2} p_N(t, z, z) = 2[1 - \tfrac{1}{4}\sqrt{\pi t}\,\mathrm{tr}\, H] + O(t).$$

Proposition 4 is proved.

6. Determination of the constants C and D

From the last section we see that direct computation of the coefficients C and D involves a large number of definite integrals. We will determine C and D indirectly by showing that A, B, C, D are universal constants, i.e., they do not depend on the dimension n.

To prove this assertion, consider the symbolic expression

$$g^Z(x) = I + 2Z_1|x^1| + Z_{11}|x^1|^2 + 2Z_{1k}|x^1|x^k - \tfrac{1}{3}Z_{kl}x^k x^l + O(|x|^3). \tag{6.1}$$

Clearly we obtain the metric matrix expansion by the substitutions

$$Z_1 = H, \quad Z_{11} = -R_{1\cdot 1\cdot} + H^2, \quad Z_{1k} = \partial_k H, \quad Z_{kl} = \{Z_{ikjl} = R^{\partial\Omega}_{ikjl}\}.$$

In the computation of the last section, besides the symmetry of these Z matrices, the only algebraic relation we use among the entries of Z's are the relations among the components of the Riemannian curvature tensor:

$$Z_{ijkj} = -Z_{jikl} = -Z_{ijkl} = Z_{klij}. \tag{6.2}$$

Now in (6.1), we regard the entries of these matrices Z_1, Z_{11}, Z_{1k}, Z_{kl} as algebraically independent variables subject only to the relations in (6.2). Note that H, H^2, $R_{1\cdot 1\cdot}$, $2\partial_k H$, $R_{\cdot k \cdot j}$ may not be algebraically independent in some special cases. For example, by Gauss's *Theorema Egregium*, we have $H_{ii}H_{jj} - H_{ij}^2 = R_{ijij}$ for $2 \le i, j \le n$. However the important fact is that the symmetry of Z matrices and (6.2) are the only algebraic relations we have used in the last section. The symbolic expansion (6.1) can be used instead of the actual expansion of the metric matrix in the computation of the last section. Let us denote the resulting a_3 and $a_3(z)$ by a_3^Z and $a_3^Z(z)$ respectively. We then have

$$a_3^Z = \int_{\partial\Omega} a_3^Z(z)\sigma(dz),$$

where $a_3^Z(z)$ are polynomials in the entries of the Z matrices. The computation in the last section shows that $a_3^Z(z)$ must have the following form

$$a_3^Z(z) = \lambda_1(\text{tr } Z_1)^2 + \lambda_2\text{tr}(Z_1)^2 + \lambda_3\text{tr } Z_{11} + \lambda_4 K^Z\,, \tag{6.3}$$

where $K^Z = \sum_{2\le i,j\le n} Z_{ijij}$. Furthermore, A, B, C, D are obtained in such way that

$$A = \lambda_4\,, \qquad B = \lambda_3\,, \qquad C = \lambda_1\,, \qquad D = \lambda_1 + \lambda_2.$$

Thus to prove A, B, C, D are universal it is enough to show that same for λ_i, $i = 1, 2, 3, 4$.

Proposition 8. *The constants λ_i, $i = 1, 2, 3, 4$ defined above are independent of the dimension.*

Proof. Let $\tilde{\lambda}_i$ be the corresponding numbers for the dimension $n+1$. Let $\tilde{z} = (z, z^{n+1})$. We then have

$$\tilde{a}_3^{\widetilde{Z}}(\tilde{z}) = \tilde{\lambda}_1(\text{tr } \widetilde{Z}_1)^2 + \tilde{\lambda}_2\text{tr}(\widetilde{Z}_1)^2 + \tilde{\lambda}_3\text{tr } \widetilde{Z}_{11} + \tilde{\lambda}_4 K^{\widetilde{Z}}. \tag{6.4}$$

Let Z^* be the matrix of size $(n+1)\times(n+1)$ obtained from $\widetilde{Z}$ by replacing the entries of the last row and the last column by zeros. The key to the present proof is that from the computation of the last section

$$a_3^{Z^*}(\tilde{z}) = a_3^Z(z). \tag{6.5}$$

On the other hand, because $\text{tr } Z^* = \text{tr } Z$ and $K^{Z^*} = K^Z$, we have by setting the last row and the last column equal to zero in (6.4) that

$$a_3^{Z^*}(z) = \tilde{\lambda}_1(\text{tr } Z_1)^2 + \tilde{\lambda}_2\text{tr}(Z_1)^2 + \tilde{\lambda}_3\text{tr } Z_{11} + \tilde{\lambda}_4 K^Z. \tag{6.6}$$

It follows from (6.2), (6.4) and (6.5) that

$$(\lambda_1 - \tilde{\lambda}_1)(\text{tr } Z_1)^2 + (\lambda_2 - \tilde{\lambda}_2)\text{tr } Z_1^2 + (\lambda_3 - \tilde{\lambda}_3)\text{tr } Z_{11} + (\lambda_4 - \tilde{\lambda}_4)K^Z = 0.$$

Since this is an identity in Z variables and the four polynomials $(\text{tr } Z_1)^2$, $\text{tr } Z_1^2$, $\text{tr } Z_{11}$, K^Z are clearly linearly independent, we obtain $\lambda_i = \tilde{\lambda}_i$, $i = 1, 2, 3, 4$. □

Now that we know that C and D do not depend on the dimension n, we can determine their values as follows:

(a) If Ω is a ball of radius one in R^2, then we have the

$$K^{\partial\Omega} = 0, \qquad \text{Ric}(n) = 0, \qquad \text{tr } H = -1, \qquad \text{tr } H^2 = 1.$$

The values of a_3 can be obtained from (1.5). We have $a_3 = 7\pi^{3/2}/32$ for the Neumann case and $a_3 = \pi^{3/2}/32$ for the Dirichlet case;

(b) If Ω is a ball of radius one in R^3 then

$$K^{\partial\Omega} = 2, \qquad \text{Ric}(n) = 0, \qquad \text{tr } H = -2, \qquad \text{tr } H^2 = 2.$$

We also have the explicit asymptotic expansions:

$$(4\pi t)^{3/2}\Theta_N(t) = \tfrac{4}{3}\pi + 2\pi^{3/2}t^{1/2} + \tfrac{8}{3}\pi t - \tfrac{13}{45}\pi t^2 + O(t^{5/2})$$

(see [Z]) and

$$(4\pi t)^{3/2}\Theta_D(t) = \tfrac{4}{3}\pi - 2\pi^{3/2}t^{1/2} + \tfrac{8}{3}\pi t - \tfrac{32}{315}\pi t^2 + O(t^{5/2})$$

(see [W]). In both cases we have $a_3 = 0$. The fact that $a_3 = 0$ for the Dirichlet case can also be seen from (1.5).

The Neumann case. (a) and (b) give us equations

$$C + D = \tfrac{7}{64}\sqrt{\pi}, \qquad A + C + 2D = 0.$$

We also know that $A = \sqrt{\pi}/12$. Hence

$$C = \tfrac{29}{96}\sqrt{\pi}, \qquad D = -\tfrac{37}{192}\sqrt{\pi}.$$

The Dirichlet case. The two equations are

$$C + D = \tfrac{1}{64}\sqrt{\pi}, \qquad A + C + 2D = 0.$$

In the present case $A = -\sqrt{\pi}/12$. Hence

$$C = -\tfrac{5}{96}\sqrt{\pi}, \qquad D = \tfrac{13}{192}\sqrt{\pi}.$$

7. Localization principle

The following theorem is referred to as the localization principle.

Theorem 9. *Suppose that g_1, g_2 are two smooth Riemannian metrics on R^n which coincide on a neighborhood U of the origin O. Let $p_1(t, x, y)$ and $p_2(t, x, y)$ be the heat kernel associated with the Laplace-Beltrami operators Δ_1 and Δ_2 of the metrics g_1 and g_2, respectively. Then for any smaller neighborhood U_1 of O with $\overline{U}_1 \subset U$, there exist positive constants δ and t_0 such that*

$$\forall (t, x, y) \in (0, t_0) \times \overline{U}_1 \times \overline{U}_1, \qquad |p_1(t, x, y) - p_2(t, x, y)| \le e^{-\delta/t}. \quad \square$$

This is a well-known theorem and various existing proofs of this theorem involves ideas from probability theory in one way or another. We refer to [M] for one of such proofs.

We can paraphrase the localization principle as follows: Since the difference between $p_1(t, x, y)$ and $p_2(t, x, y)$ is exponentially small, the asymptotic properties of these two heat kernels in powers of t are the same. Therefore, when studying such asymptotic properties at a fixed point O, we may arbitrarily alter the metric outside a neighborhood of O without affecting final results.

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