ASYMPTOTICS OF THE HEAT CONTENT FOR DOMAINS WITH SMOOTH BOUNDARY

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We give a recursive algorithm for the computation of the complete asymptotic series, for small time, of the amount of heat inside a domain with smooth boundary in a Riemannian manifold; we consider arbitrary smooth initial data, and we impose Dirichlet condition on the boundary. Our coefficients are given in terms of the algebra of differential operators generated by the Laplacian of the manifold, and by an operator of order one written in terms of the mean curvature of the hypersurfaces parallel to the boundary.

Introduction

Let Ω be a domain in a complete Riemannian manifold. We assume $\bar\Omega$ compact and $\partial\Omega$ smooth. Let $u(t,x)$ be the solution of the heat equation on Ω, satisfying Dirichlet boundary conditions, and unit initial conditions: $u(0,x)=1$ for all $x\in\Omega$. Fix $\phi\in C^\infty(\bar\Omega)$, and define:

$$H(t)=\int_\Omega u(t,x)\phi(x)\,dx$$

$H(t)$ is the amount of heat inside Ω at time t, given that the initial temperature at time $t=0$, at the point $x\in\Omega$, is $\phi(x)$, and assuming that the boundary of Ω is kept at zero temperature at all times.

As $t\to 0$, there exists an asymptotic series:

$$\int_\Omega u(t,x)\phi(x)\,dx\sim\int_\Omega\phi-\sum_{k=1}^\infty\beta_k(\phi)\cdot t^{k/2} \tag{1}$$

The aim of this paper is to give a recursive formula which computes the coefficient $\beta_k(\phi)$ for all $k\geq 1$.

For domains in $\mathbf{R}^m$, $\beta_1(1)$ was first computed in [2], and $\beta_2(1)$ was computed in [5]: both computations use probabilistic methods. $\beta_1(1)$ and $\beta_2(1)$ were computed for the upper hemisphere of a sphere in [1]; then, van den Berg and Gilkey (in [4]) established the existence of the asymptotic series, and proceeded to compute the coefficients $\beta_k(\phi)$ up to $k=4$ for domains in Riemannian manifolds, and up to $k=7$ for balls in $\mathbf{R}^n$, when $\phi=1$. Their calculation use the functorial properties of β_k: in fact the method extends to operators of Laplace type, and to Neumann boundary conditions (in which case, the first six terms of the expansion are calculated, see [3], [10]).

If Ω is a polyhedron in $\mathbf{R}^m$, there is also an asymptotic expansion of the type:

$$\int_\Omega u(t,x)\,dx\sim\mathrm{vol}(\Omega)+\beta_1(1)\cdot t^{1/2}+\beta_2(1)\cdot t+O(t^{\frac{3}{2}})$$

$\beta_1(1)$ and $\beta_2(1)$ were computed in [6] for polygonal domains in the plane, and in [14] for convex polyhedral bodies in $\mathbf{R}^m$. These results do not follow trivially from the smooth case; in fact $\beta_2(1)$ does not pass to the limit under smooth approximations of the polyhedron.

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Let us then assume that $\partial\Omega$ is smooth. We show that, for each $k \geq 1$, $\beta_k(\phi)$ is given by integration, over $\partial\Omega$ and for the induced Riemannian measure, of the function $D_k\phi$, where D_k is a differential operator, acting on $C_c^\infty(U)$ (U is a fixed neighborhood of $\partial\Omega$ in Ω) and belonging to the algebra $\mathcal{A}$ generated by the Laplacian Δ of the manifold, and by the operator N, of order 1, defined by the formula:

$$N\phi = 2\nabla\phi \cdot \nabla\rho - \phi\Delta\rho \tag{2}$$

where $\rho : \Omega \to \mathbf{R}$ is the *distance function from* $\partial\Omega$ (since $\partial\Omega$ is assumed to be smooth, the distance function ρ is $C^\infty-$ smooth in a neighborhood of $\partial\Omega$). We observe that the coefficients $\beta_k(\phi)$, for $k \geq 1$, depend only on the behavior of the initial data ϕ near the boundary of Ω, hence they really give invariants for the immersion of $\partial\Omega$ in Ω (the interior invariants β_k^{int} (in the sense of [4]) are zero in our case for $k \geq 1$); in particular, domains which are locally isometric near the respective boundaries give rise to the same sequence of coefficients $\beta_k(1)$, for $k \geq 1$.

About the operators D_k, we show that each D_k is homogeneous of order $k-1$ in N and Δ, and we give a recursive formula which expresses D_k in terms of D_i, $i \leq k-1$. Since $\Delta\rho$, at its C^∞-points, gives the trace of the second fundamental form of the level hypersurfaces of the distance function ρ (the parallel manifolds of $\partial\Omega$), each $D_k\phi$ could be expressed in terms of the classical invariants: namely, the curvature tensor and its covariant derivatives, and the second fundamental form and its covariant derivatives. In this way one can recover the coefficients of (1) up to $\beta_4(\phi)$ as presented in [4] (our $\beta_k(\phi)$ corresponds to $-\beta_k(\phi,1)$ in [4]).

Main theorem. *For each $k \geq 1$, there exists a homogeneous polynomial D_k of degree $k-1$ in the operators N and Δ such that:*

$$\beta_k(\phi) = \int_{\partial\Omega} D_k\phi$$

Let the families of operators of type R and S be defined inductively by:

$$\begin{cases} R_{kj} = -(N^2 + \Delta)R_{k-1,j} + NS_{k-1,j} \\ S_{kj} = NR_{k-1,j-1} + \Delta N R_{k-1,j} - \Delta S_{k-1,j} \\ R_{00} = Id, \quad S_{00} = 0 \quad R_{kj} = 0 \quad if \quad j < 0 \end{cases}$$

and set: $\{a,b\} = \dfrac{\Gamma(a+b+1/2)}{(a+b)!\Gamma(a+1/2)}$, $Z_{n+1} = \sum_{j=0}^{n}\{n+1, j-1\}R_{n+j,j}$, *and* $\alpha_k = \sum_{j=0}^{k+1}\{k,j\}S_{k+j,j}$. *Then the following recursive formulas hold:*

$$\begin{aligned} D_1 &= \frac{2}{\sqrt{\pi}} Id \\ D_{2n} &= \frac{1}{\sqrt{\pi}} \sum_{i=1}^{n} \frac{\Gamma(i+\frac{1}{2})\Gamma(n-i+\frac{1}{2})}{n!} D_{2i-1}\alpha_{n-i} \\ D_{2n+1} &= \frac{1}{\sqrt{\pi}} Z_{n+1} + \frac{1}{\sqrt{\pi}} \sum_{i=1}^{n} \frac{i!\Gamma(n-i+\frac{1}{2})}{\Gamma(n+\frac{3}{2})} D_{2i}\alpha_{n-i} \end{aligned}$$

We give below the explicit expression of the operators $D_1, \ldots, D_8$:

$$
\begin{aligned}
D_1 &= \frac{2}{\sqrt{\pi}} Id \\
D_2 &= \frac{1}{2} N \\
D_3 &= \frac{1}{6\sqrt{\pi}}(N^2 - 4\Delta) \\
D_4 &= -\frac{1}{16}(\Delta N + 3N\Delta) \\
D_5 &= -\frac{1}{240\sqrt{\pi}}(N^4 + 16N^2\Delta + 8N\Delta N - 48\Delta^2) \\
D_6 &= \frac{1}{768}(\Delta N^3 - N^3\Delta + N\Delta N^2 - N^2\Delta N + 40N\Delta^2 + 8\Delta^2 N + 16\Delta N\Delta) \\
D_7 &= \frac{1}{6720\sqrt{\pi}}(N^6 + 120N^2\Delta^2 + 4N^3\Delta N + 4N^2\Delta N^2 + 4N\Delta N^3 + 72(N\Delta)^2 + 40N\Delta^2 N + 8N^4\Delta + \\
&\quad + 8\Delta N^2\Delta + 8(\Delta N)^2 - 8\Delta^2 N^2 - 320\Delta^3) \\
D_8 &= -\frac{1}{24576}(40\Delta^3 N + 8\Delta N^3\Delta + 280N\Delta^3 + 8N\Delta^2 N^2 - 8N^2\Delta^2 N + 72\Delta^2 N\Delta + 120\Delta N\Delta^2 + \\
&\quad + 4\Delta^2 N^3 + 4\Delta N\Delta N^2 + 4\Delta N^2\Delta N + 4N\Delta N^2\Delta - 12N^3\Delta^2 + \Delta N^5 - N^4\Delta N - N^5\Delta)
\end{aligned}
$$

The case $\phi = 1$ is of particular significance, since then:

$$
H(t) = \int_{\Omega\times\Omega} k(t,x,y)\, dx\, dy
$$

$k(t,x,y)$ being the Dirichlet heat kernel of Ω. Since $\Delta 1 = 0$, and $N1 = -\Delta\rho$, the coefficients $\beta_1(1), \dots, \beta_8(1)$ are given by:

$$
\begin{aligned}
\beta_1(1) &= \frac{2}{\sqrt{\pi}} vol(\partial\Omega) \\
\beta_2(1) &= -\frac{1}{2}\int_{\partial\Omega} \Delta\rho \\
\beta_3(1) &= -\frac{1}{6\sqrt{\pi}}\int_{\partial\Omega} N\Delta\rho \\
\beta_4(1) &= \frac{1}{16}\int_{\partial\Omega} \Delta^2\rho \\
\beta_5(1) &= \frac{1}{240\sqrt{\pi}}\int_{\partial\Omega} (N^3 + 8N\Delta)\Delta\rho \\
\beta_6(1) &= -\frac{1}{768}\int_{\partial\Omega} (\Delta N^2 + N\Delta N - N^2\Delta + 8\Delta^2)\Delta\rho \\
\beta_7(1) &= -\frac{1}{6720\sqrt{\pi}}\int_{\partial\Omega} (N^5 + 4N^3\Delta + 4N^2\Delta N + 4N\Delta N^2 + 40N\Delta^2 + 8\Delta N\Delta - 8\Delta^2 N)\Delta\rho \\
\beta_8(1) &= \frac{1}{24576}\int_{\partial\Omega} (40\Delta^3 + 8N\Delta^2 N - 8N^2\Delta^2 + 4\Delta^2 N^2 + 4\Delta N\Delta N + 4\Delta N^2\Delta + \Delta N^4 - N^4\Delta)\Delta\rho
\end{aligned}
$$

and in general $\beta_k(1)$, for $k \geq 2$, is given by integration on $\partial\Omega$ of a differential operator of order $k-2$ in N and Δ, applied to $\Delta\rho$.

The method we use is to reduce the study of (1) to a *one-dimensional* problem. It could be summarized as follows. First observe that $\sum_{k=1}^{\infty} \beta_k(\phi)$ is the asymptotic series, as $t \to 0$, of the function:

$$I\phi(t) = \int_\Omega (1-u(t,x))\phi(x)\,dx$$

We introduce an auxiliary variable $r \in [0,\infty)$ and let:

$$I\phi(t,r) = \int_{\Omega(r)} (1-u(t,x))\phi(x)\,dx$$

where $\Omega(r) = \{x \in \Omega : d(x,\partial\Omega) > r\}$ is the *parallel domain at distance r from $\partial\Omega$*. By the so-called *principle of not feeling the boundary* , in order to examine the asymptotic behavior of $I\phi(t)$ as $t \to 0$, we can assume that ϕ is supported in a neighborhood U of $\partial\Omega$: in that case, $I\phi(t,r)$ is *smooth* in both variables, and satisfies a one-dimensional heat equation on the half-line of type:

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial t}\right) I\phi = L^1 I\phi$$

where:

$$L^1 I\phi(t,r) = \int_{\rho^{-1}(r)} (1-u(t,x))N\phi(x)\,dx - \int_{\Omega(r)} (1-u(t,x))\Delta\phi(x)\,dx \tag{3}$$

By Duhamel principle, iterated infinitely many times, we can then represent $I\phi(t,0)$ in terms of the derivatives of the one-dimensional heat kernel $e(t,r,0) = \frac{1}{\sqrt{\pi t}} e^{-r^2/4t}$ and the powers L^k of the heat operator $L = -\frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial t}$ applied to $I\phi$. The algebraic relations coming from this process will lead to the recursive formulas of the main Theorem, and the form of (3) roughly explains why the operators D_k are generated by N and Δ.

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The algorithm

We first introduce the distance function from the boundary: $\rho(x) = dist(x,\partial\Omega)$ (for complete details, see [14]). ρ is Lipschitz on Ω, and is C^∞-smooth on the set $\Omega \setminus Cut(\partial\Omega)$, where $Cut(\partial\Omega)$ is the cut-locus of the normal exponential map of $\partial\Omega$. $Cut(\partial\Omega)$ has zero measure in Ω, and at all C^∞-points of ρ we have $\|\nabla\rho\| = 1$. Fix a smooth map v on Ω, and define:

$$F(r) = \int_{\Omega(r)} v(x)\,dx$$

where $\Omega(r) = \{x \in \Omega : \rho(x) > r\}$ is the parallel domain at distance r from $\partial\Omega$. Then F is Lipschitz on $(0,\infty)$, and we have (see Theorem 2.8 in [14]):

$$F''(r) = -\int_{\Omega(r)} \Delta v(x)\,dx + \rho_*(v\Delta\rho)(r) \tag{4}$$

in the sense of distributions on $(0,\infty)$: here $\Delta\rho$ is the distributional Laplacian of ρ (it is, in fact, a measure) and $\rho_*(v\Delta\rho)$ is the measure on $(0,\infty)$ which is the push-forward of $v\Delta\rho$ by ρ. However in this paper we are going to apply (4) only for r in an arbitrarily small neighborhood of 0. If we let R_{inj} denote the injectivity radius of $\partial\Omega$ in Ω, then ρ is C^∞-smooth on the strip $\{x \in \Omega : \rho(x) < R_{inj}\}$, and so $F(r)$ is also C^∞-smooth on $(0, R_{inj})$, and, on this interval, we have:

$$F''(r) = -\int_{\Omega(r)} \Delta v(x)\, dx + \int_{\rho^{-1}(r)} v(y)\Delta\rho(y)\, dy \tag{5}$$

where dy is the induced Riemannian measure on the submanifold $\rho^{-1}(r)$. Finally, at all C^∞-points x of ρ, $\Delta\rho(x)$ gives the trace of the second fundamental form of the level submanifold $\rho^{-1}(\rho(x))$, with respect to the unit normal vector $\nu = \nabla\rho$.

In what follows $u(t,x)$ will always denote the following solution of the heat equation on Ω:

$$\begin{cases} \left(\Delta + \dfrac{\partial}{\partial t}\right) u = 0 \\ u(0,x) = 1 \qquad \text{for all} \quad x \in \Omega \\ u(t,y) = 0 \qquad \text{for all} \quad t > 0, \quad y \in \partial\Omega \end{cases}$$

Note that $u(t,x) = \int_\Omega k(t,x,y)\, dy$, where $k(t,x,y)$ is the Dirichlet heat kernel of the domain Ω.

So fix $\phi \in C^\infty(\bar{\Omega})$. Our aim is to compute the asymptotic series $\sum_{k=1}^\infty \beta_k(\phi) \cdot t^{k/2}$ of the function:

$$I\phi(t) = \int_\Omega (1 - u(t,x))\phi(x)\, dx$$

as $t \to 0$. We first prove the following Proposition:

Proposition 6. *Let $\phi, \phi' \in C^\infty(\bar{\Omega})$. If $\phi = \phi'$ on a neighborhood U of $\partial\Omega$, then $\beta_k(\phi) = \beta_k(\phi')$ for all $k \geq 1$.*

Proof. See Appendix A.

For the rest of the paper, we fix $a < R_{inj}$, and let U be the strip (tubular neighborhood) of width a around $\partial\Omega$:

$$U = \{x \in \bar{\Omega} : \rho(x) < a\}$$

Thanks to Proposition 6, *we can assume from now on that ϕ is supported on U* (if not, we can reduce to this situation by a partition of unity argument).

Notation. We introduce the following symbolism. For $\phi \in C_c^\infty(U)$, define:

$$I\phi(t,r) = \int_{\Omega(r)} (1 - u(t,x))\phi(x)\, dx$$

$$\Lambda\phi(t,r) = \int_{\rho^{-1}(r)} (1 - u(t,x))\phi(x)\, dx$$

Since U does not intersect the cut-locus of $\partial\Omega$ in Ω, we see that $I\phi(t,r)$ and $\Lambda\phi(t,r)$ are *smooth* on $(0,\infty) \times [0,\infty)$. Our notation stresses the role of ϕ, and in fact it will be convenient for us to regard I and Λ as operators taking $\phi \in C_c^\infty(U)$ to $I\phi$ and $\Lambda\phi$, both in $C^\infty((0,\infty) \times [0,\infty))$ (and supported for $r < a$). Note that $\dfrac{\partial}{\partial r} I = -\Lambda$.

The computation of the asymptotic series of the heat content relies on an iteration of Duhamel principle (see Lemma 9 below). In order to be able to apply Lemma 9, we will need to consider the following approximation of the temperature function $u(t,x)$: for $0 < \epsilon < a$, let $u_\epsilon(t,x)$ be the solution of the heat equation on Ω, satisfying Dirichlet boundary conditions, and having initial conditions:

$$u_\epsilon(0,x) = \begin{cases} 1 & \text{if} \quad \rho(x) > \epsilon \\ 0 & \text{otherwise} \end{cases}$$

Since the initial conditions of u_ϵ tend to the initial conditions of u as $\epsilon \to 0$, in the sense of distributions, we see that, for fixed (t,x):

$$\lim_{\epsilon\to 0} u_\epsilon(t,x) = u(t,x)$$

Then let:

$$I_\epsilon\phi(t,r) = \int_{\Omega(r)} (1-u_\epsilon(t,x))\phi(x)\,dx$$
$$\Lambda_\epsilon\phi(t,r) = \int_{\rho^{-1}(r)} (1-u_\epsilon(t,x))\phi(x)\,dx$$

By Lebesgue bounded convergence theorem:

$$I\phi(t) \equiv \int_\Omega (1-u(t,x))\phi(x)\,dx = \lim_{\epsilon\to 0} I_\epsilon\phi(t,0)$$

Recall that $I_\epsilon\phi(t,r)$ is C^∞-smooth in (t,r) for $t>0$ and $r\geq 0$. For any j we regard $\frac{\partial^j}{\partial t^j} I_\epsilon\phi(0,r)$ as a distribution on $[0,\infty)$ (it is in fact supported on the interval $[0,a)$) and set, for $\psi \in C^\infty([0,\infty))$:

$$\int_0^\infty \frac{\partial^j}{\partial t^j} I_\epsilon\phi(0,r)\psi(r)\,dr = \lim_{t\to 0}\int_0^\infty \frac{\partial^j}{\partial t^j} I_\epsilon\phi(t,r)\psi(r)\,dr$$

We also set:

$$\frac{\partial^j}{\partial t^j} I_\epsilon\phi(0,0) = \lim_{t\to 0}\frac{\partial^j}{\partial t^j} I_\epsilon\phi(t,0)$$

Similar definitions hold for the function $\Lambda_\epsilon\phi$. All these limits will be evaluated in Lemma 15.

We then introduce the algebra $\mathcal{A}$ of all differential operators acting on $C_c^\infty(U)$, generated by the Laplacian Δ, and by the operator N, which takes ϕ to $2\frac{\partial\phi}{\partial\nu} - \phi\Delta\rho$, where $\nu = \nabla\rho$ is the unit vector, normal to the level hypersurfaces of the distance function ρ (the parallel hypersurfaces). The families of operators in $\mathcal{A}$, of type P,Q,R,S are defined inductively by the formulas:

(7)
$$\begin{cases} P_{kj} = -(N^2+\Delta)P_{k-1,j} + NQ_{k-1,j} \\ Q_{kj} = NP_{k-1,j-1} + \Delta NP_{k-1,j} - \Delta Q_{k-1,j} \\ P_{00} = 0, \quad Q_{00} = Id, \quad P_{kj} = 0 \quad \text{if} \quad j<0 \end{cases}$$

and:

(8)
$$\begin{cases} R_{kj} = -(N^2+\Delta)R_{k-1,j} + NS_{k-1,j} \\ S_{kj} = NR_{k-1,j-1} + \Delta NR_{k-1,j} - \Delta S_{k-1,j} \\ R_{00} = Id, \quad S_{00} = 0, \quad R_{kj} = 0 \quad \text{if} \quad j<0 \end{cases}$$

The operator P_{kj} has order $2(k-j)-1$, and vanishes for $2j>k-1$; the operators Q_{kj} and R_{kj} have order $2(k-j)$ and vanish for $2j>k$, and the operator S_{kj} has order $2(k-j)+1$ and vanishes for $2j>k+1$.

As mentioned in the Introduction, our method is based on a reduction to a one dimensional problem; the following lemma is an iterated version of Duhamel principle on the half-line, and is the technical tool upon which our computation is based. So let $L = -\frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial t}$ be the heat operator, and let $e(t,r,s)$ denote the *heat kernel of the half-line* $(0,\infty)$ subject to Neumann boundary conditions at $r=0$; explicitly:

$$e(t,r,s) = \frac{1}{\sqrt{4\pi t}}\left(e^{-(r+s)^2/4t} + e^{-(r-s)^2/4t}\right)$$

and in particular:

$$e(t,r,0) = \frac{1}{\sqrt{\pi t}} e^{-r^2/4t}$$

Lemma 9 (Iterated Duhamel principle).

Let $F(t,r)$ be smooth on $(0,\infty)\times[0,\infty)\to\mathbf{R}$, and assume that:

(i) $L^kF(0,r) = \lim_{t\to 0} L^kF(t,r)$ *exists in the sense of distributions for each* $k\geq 0$*;*

(ii) *As* $t\to 0$*, both* $L^kF(t,0)$ *and* $\frac{\partial}{\partial r}L^kF(t,0)$ *converge to a finite limit, for each* $k\geq 0$*.*

Then, for all $m\in\mathbf{N}$*, and* $t>0$*:*

$$F(t,0) = \sum_{k=0}^m \frac{t^k}{k!}\int_0^\infty e(t,r,0)L^kF(0,r)\,dr - \frac{1}{\sqrt{\pi}}\sum_{k=0}^m\frac{1}{k!}\int_0^t \frac{\partial}{\partial r}L^kF(\tau,0)(t-\tau)^{k-1/2}\,d\tau + \\ + \frac{1}{m!}\int_0^t\int_0^\infty e(t-\tau,r,0)L^{m+1}F(\tau,s)(t-\tau)^m\,ds\,d\tau$$

Proof. Given our assumptions on F, the classical Duhamel principle holds for every L^mF, in the sense that, for all $t>0$, and $r\geq 0$:

(10)

$$L^mF(t,r) = \int_0^\infty e(t,r,s)L^mF(0,s)\,ds - \int_0^t \frac{\partial}{\partial r}L^mF(\tau,0)e(t-\tau,r,0)\,d\tau + \int_0^t\int_0^\infty e(t-\tau,r,s)L^{m+1}F(\tau,s)\,ds\,d\tau$$

Taking $r=0$, we see that the lemma holds for $m=0$. To lighten notation, we introduce the (heat) semigroup operator β_t of the half-line, acting on the distribution U by the formula:

$$\beta_tU(r) = \int_0^\infty e(t,r,s)U(s)\,ds$$

The semigroup property of β_t states that: $\beta_{t+s} = \beta_t\circ\beta_s$ for all $t,s\geq 0$. We also let: $\bar\beta_tU = \beta_tU(0)$, so that $\bar\beta_t\circ\beta_s = \bar\beta_{t+s}$. Finally, we write F_t for the function $F_t(r) = F(t,r)$.

We now assume that the formula in (ii) holds for $m-1$. The lemma will follow if we show that, in our short notation:

(11) $$\int_0^t \bar\beta_{t-\tau}(L^mF)_\tau\frac{(t-\tau)^{m-1}}{(m-1)!}\,d\tau = \frac{t^m}{m!}\bar\beta_t(L^mF)_0 \\ + \int_0^t\bar\beta_{t-\tau}(L^{m+1}F)_\tau\frac{(t-\tau)^m}{m!}\,d\tau - \frac{1}{\sqrt{\pi}}\int_0^t\frac{\partial}{\partial r}(L^mf)_\tau(0)\frac{(t-\tau)^{m-1/2}}{m!}\,d\tau$$

From Duhamel principle applied to L^mF (see (10)):

$$(L^mF)_\tau = \beta_\tau(L^mF)_0 + \int_0^\tau\beta_{\tau-\mu}(L^{m+1}F)_\mu\,d\mu - \int_0^\tau\frac{\partial}{\partial r}(L^mF)_\mu(0)\beta_{\tau-\mu}\delta_0\,d\mu$$

where δ_0 is the Dirac distribution at $r=0$. When we plug $(L^mF)_\tau$ in the left-hand side of (11), we obtain three terms. We examine each of them separately.

Since $\bar\beta_{t-\tau}\,\beta_\tau = \bar\beta_t$, the first term becomes $\frac{t^m}{m!}\bar\beta_t(L^mF)_0$.

When we plug $\int_0^\tau\beta_{\tau-\mu}(L^{m+1}F)_\mu\,d\mu$ into the left-hand side of (11), we get:

$$\frac{1}{(m-1)!}\int_0^t\int_0^\tau (t-\tau)^{m-1}\bar\beta_{t-\tau}\beta_{\tau-\mu}(L^{m+1}F)_\mu \, d\mu \, d\tau$$

using the semigroup property of β_t, and switching order of integration , we obtain:

$$\frac{1}{(m-1)!}\int_0^t\int_\mu^t (t-\tau)^{m-1}\bar\beta_{t-\mu}(L^{m+1}F)_\mu \, d\tau \, d\mu = \int_0^t \bar\beta_{t-\mu}(L^{m+1}F)_\mu \frac{(t-\mu)^m}{m!}\, d\mu$$

Finally, we plug $-\int_0^\tau \frac{\partial}{\partial r}(L^m F)_\mu(0)\beta_{\tau-\mu}\delta_0 \, d\mu$ into the left-hand side of (11), and get:

$$-\int_0^t\int_0^\tau \frac{(t-\tau)^{m-1}}{(m-1)!}\frac{\partial}{\partial r}(L^m F)_\mu(0)(\bar\beta_{t-\mu}\delta_0)\, d\mu \, d\tau$$

we switch order of integration, and we observe that: $\bar\beta_{t-\mu}\delta_0 = \frac{1}{\sqrt{\pi}}(t-\mu)^{-1/2}$. The expression becomes:

$$-\frac{1}{\sqrt{\pi}}\int_0^t \frac{\partial}{\partial r}(L^m F)_\mu(0)\frac{(t-\mu)^{m-1/2}}{m!}\, d\mu$$

We add-up the three terms, thus verifying (11). Proof is complete. □

The next lemma shows how the operators $L^k I$ and $L^k \Lambda$ can be expressed in terms of the algebra $\mathcal{A}$, and partial differentiation with respect to time. The same relations hold replacing $L^k I$ and $L^k\Lambda$ by $L^k I_\epsilon$ and $L^k\Lambda_\epsilon$, and in fact they hold if, in the definition of $I\phi$ and $\Lambda\phi$, one replaces $1-u$ by any solution of the heat equation on Ω.

Lemma 12.
(i) $LI = \Lambda N - I\Delta$
(ii) $L\Lambda = -\Lambda(N^2+\Delta) + I\Delta N + \frac{\partial}{\partial t} IN$
and for all $k \in \mathbf{N}$:

(iii)
$$L^k I = \sum_{j=0}^{\infty}\frac{\partial^j}{\partial t^j}\left(\Lambda P_{kj} + IQ_{kj}\right)$$
$$L^k \Lambda = \sum_{j=0}^{\infty}\frac{\partial^j}{\partial t^j}\left(\Lambda R_{kj} + IS_{kj}\right)$$

where the operators of type P, Q, R, S belong to $\mathcal{A}$ and have been defined in (7) and (8).
Therefore, both sums in (iii) are finite (in fact in the first $j \le [\frac{k}{2}]$ and in the second $j \le [\frac{k+1}{2}]$)

Proof. By formula (4):

$$-\frac{\partial^2}{\partial r^2} I\phi(t,r) = -\frac{\partial^2}{\partial r^2}\int_{\Omega(r)}(1-u)\phi$$
$$= \int_{\Omega(r)}\Delta((1-u)\phi) - \int_{\rho^{-1}(r)}(1-u)\phi\Delta\rho$$

By Green's formulas, the first integral equals:

$$2\int_{\rho^{-1}(r)}(1-u)\nabla\phi\cdot\nabla\rho - \int_{\Omega(r)}(1-u)\Delta\phi + \int_{\Omega(r)}\phi\Delta(1-u)$$

Therefore:

$$-\frac{\partial^2}{\partial r^2} I\phi = \Lambda N\phi - I\Delta\phi - \frac{\partial}{\partial t} I\phi \tag{13}$$

Adding $\frac{\partial}{\partial t} I\phi$ to both sides, we obtain (i). As for (ii), observe that, since $\frac{\partial}{\partial r} I = -\Lambda$, (13) can be re-written:

$$\frac{\partial}{\partial r}\Lambda = \Lambda N - I\Delta - \frac{\partial}{\partial t} I \tag{14}$$

Now apply $\frac{\partial}{\partial r}$ to both sides of (14); since $\frac{\partial}{\partial r}\frac{\partial}{\partial t} = \frac{\partial}{\partial t}\frac{\partial}{\partial r}$, we obtain: $\frac{\partial^2}{\partial r^2}\Lambda = \frac{\partial}{\partial r}\Lambda N + \Lambda\Delta + \frac{\partial}{\partial t}\Lambda$

We change sign, use (14) again, add $\frac{\partial}{\partial t}\Lambda$ to both sides and get (ii). As for the other assertions in the lemma, they can be easily verified by induction on k. □

We cannot immediately apply the iterated Duhamel principle to $I\phi(t,r)$, because $I\phi$, for $k > 2$, does not satisfy the conditions (i) and (ii) of Lemma 9. However, the conditions are satisfied by $I_\epsilon\phi$, as the next lemma shows. The idea is then to apply Lemma 9 to $I_\epsilon\phi$, obtain an asymptotic series, and then pass to the limit as $\epsilon \to 0$.

Thanks to Lemma 12, it is enough to check the conditions (i) and (ii) of Lemma 9 for functions of type: $\frac{\partial^j}{\partial t^j} I_\epsilon\phi(t,r)$ and $\frac{\partial^j}{\partial t^j}\Lambda_\epsilon\phi(t,r)$.

Lemma 15. *Let $\psi \in C^\infty([0,\infty))$, and set $\psi^{(-1)}(r) = \int_0^r \psi(s)\,ds$. Denote by $\Omega'(\epsilon)$ the tubular neighborhood of $\partial\Omega$ of radius ϵ: $\Omega'(\epsilon) = \{x \in \Omega : \rho(x) < \epsilon\}$. Then:*

(i) $$\int_0^\infty \frac{\partial^j}{\partial t^j}\Lambda_\epsilon\phi(0,r)\psi(r)\,dr = \begin{cases} \int_{\Omega'(\epsilon)} \phi(\psi\circ\rho) & \text{if } j = 0 \\ (-1)^{j-1}\int_{\Omega(\epsilon)} \Delta^j(\phi(\psi\circ\rho)) & \text{if } j \geq 1 \end{cases}$$

(ii) $$\int_0^\infty \frac{\partial^j}{\partial t^j} I_\epsilon\phi(0,r)\psi(r)\,dr = \begin{cases} \int_{\Omega'(\epsilon)} \phi(\psi^{(-1)}\circ\rho) & \text{if } j = 0 \\ (-1)^{j-1}\int_{\Omega(\epsilon)} \Delta^j(\phi(\psi^{(-1)}\circ\rho)) & \text{if } j \geq 1 \end{cases}$$

(iii) $$\frac{\partial^j}{\partial t^j}\Lambda_\epsilon\phi(t,0) = \begin{cases} \int_{\partial\Omega} \phi & \text{if } j = 0 \\ 0 & \text{if } j \geq 1 \end{cases} \qquad \textit{for all} \quad t \geq 0$$

(iv) $$\frac{\partial^j}{\partial t^j} I_\epsilon\phi(0,0) = \begin{cases} \int_{\Omega'(\epsilon)} \phi & \text{if } j = 0 \\ (-1)^{j-1}\int_{\Omega(\epsilon)} \Delta^j\phi \end{cases}$$

Proof. The lemma is a consequence of the fact that, if $\phi \in C^\infty(\bar{\Omega})$, then:

(16) $$\lim_{t\to 0}\int_\Omega \phi(x)\Delta^j u_\epsilon(t,x)\,dx = \int_{\Omega(\epsilon)} \Delta^j \phi$$

To see that, write:

$$\int_\Omega \phi(x)\Delta^j u_\epsilon(t,x)\,dx = \int_\Omega \alpha_1(x)\phi(x)\Delta^j u_\epsilon(t,x)\,dx + \int_\Omega \alpha_2(x)\phi(x)\Delta^j u_\epsilon(t,x)\,dx$$

where $supp\alpha_1 \subseteq \Omega'(\epsilon/2)$, $supp\alpha_2 \subseteq \Omega$, and $\alpha_2 = 1$ on $\Omega(\epsilon)$. Since, as $t \to 0$, $u_\epsilon(t,\cdot)$ converges uniformly to 0, together with all its derivatives, on $\Omega'(\epsilon/2)$, we see that the first integral tends to zero with t; and as $\alpha_2\phi$ is compactly supported inside Ω, the second integral converges to $\int_{\Omega(\epsilon)} \Delta^j(\alpha_2\phi) = \int_{\Omega(\epsilon)} \Delta^j\phi$.

(i)-(iv) are clear for $j = 0$. Now since, for $j \geq 1$, $\frac{\partial^j}{\partial t^j}(1 - u_\epsilon(t,x)) = (-1)^{j-1}\Delta^j u_\epsilon(t,x)$, and: $\frac{\partial^j}{\partial t^j} I_\epsilon\phi(t,0) = (-1)^{j-1}\int_\Omega \Delta^j u_\epsilon(t,x)\phi(x)\,dx$, (iv) follows immediately from (16). (iii) is immediate from the Dirichlet conditions imposed on u_ϵ. We have, by the formula of co-area (see [7]):

$$\begin{aligned}\int_0^\infty \frac{\partial^j}{\partial t^j}\Lambda_\epsilon\phi(t,r)\psi(r)\,dr &= (-1)^{j-1}\int_0^\infty \psi(r)\int_{\rho^{-1}(r)} (\Delta^j u_\epsilon)\phi\,dr \\ &= (-1)^{j-1}\int_\Omega (\Delta^j u_\epsilon)\phi\cdot(\psi\circ\rho)\end{aligned}$$

and (i) also follows from (16) by letting $t \to 0$. Finally, (ii) follows from (i) by integration by parts. ☐

Lemma 17. *Let $\phi \in C_c^\infty(U)$. Then, for each $m \in \mathbf{N}$, and for each $t > 0$:*

$$I\phi(t,0) = Z^{(m)}(t) + \frac{1}{\sqrt{\pi}}B^{(m)}(t) + O(t^{\frac{m+1}{2}})$$

where:

$$\begin{aligned}Z^{(m)}(t) &= \lim_{\epsilon\to 0}\sum_{k=0}^m \frac{t^k}{k!}\int_0^\infty e(t,r,0)L^k I_\epsilon\phi(0,r)\,dr \\ B^{(m)}(t) &= \lim_{\epsilon\to 0}\sum_{k=0}^m \frac{1}{k!}\int_0^t L^k\Lambda_\epsilon\phi(\tau,0)(t-\tau)^{k-1/2}\,d\tau\end{aligned}$$

Proof. We apply the iterated Duhamel principle (Lemma 9) to $I_\epsilon\phi(t,r)$ and then let $\epsilon \to 0$; the lemma will follow if we show that:

$$\lim_{\epsilon\to 0}\int_0^t\int_0^\infty (t-\tau)^m e(t-\tau,r,0)L^{m+1}I_\epsilon\phi(\tau,r)\,dr\,d\tau$$

is $O(t^{\frac{m+1}{2}})$ as $t \to 0$. Set: $\psi_m(t,r) = t^m e(t,r,0)$.

From the expression of $L^{m+1}I_\epsilon$ given in Lemma 12 (iii), it is enough to show that, for $\phi \in C_c^\infty(U)$, and for $j \leq \frac{m+1}{2}$, (resp. $j \leq \frac{m}{2}$) the limits:

(18) $$\lim_{\epsilon\to 0}\int_0^t\int_0^\infty \psi_m(t-\tau,r,0)\frac{\partial^j}{\partial t^j}I_\epsilon\phi(\tau,r)\,dr\,d\tau$$

(19) $$\lim_{\epsilon\to 0}\int_0^t\int_0^\infty \psi_m(t-\tau,r,0)\frac{\partial^j}{\partial t^j}\Lambda_\epsilon\phi(\tau,r)\,dr\,d\tau$$

are $O(t^{\frac{m+1}{2}})$ as $t \to 0$.

We prove the assertion for (18), the one for (19) can be proved in a similar way. For $a, b \geq 0$ and such that $a + b = j \leq \frac{m+1}{2}$, set:

$$\mathcal{I}_\epsilon(a,b)(t) = \int_0^t \int_0^\infty \frac{\partial^a}{\partial \tau^a}\psi_m(t-\tau,r)\frac{\partial^b}{\partial \tau^b}I_\epsilon\phi(\tau,r)\,dr\,d\tau$$

$$\mathcal{L}_\epsilon(a,b)(t) = \int_0^\infty \frac{\partial^a}{\partial \tau^a}\psi_m(t,r)\frac{\partial^{b-1}}{\partial \tau^{b-1}}I_\epsilon\phi(0,r)\,dr$$

Now $\frac{\partial^a}{\partial t^a}\psi_m(t,r)$ is a linear combination of terms of type $r^{2i}\psi_{m-a-i}(t,r)$, for $i = 0, \ldots, a$. Therefore, for $b \geq 1$ (since then $m \geq 2a+1$): $\lim_{\tau \to t} \int_0^\infty \frac{\partial^a}{\partial \tau^a}\psi_m(t-\tau,r)\frac{\partial^{b-1}}{\partial \tau^{b-1}}I_\epsilon\phi(\tau,r)\,dr = 0$ so that, integrating by parts:

$$\mathcal{I}_\epsilon(a,b)(t) = \mathcal{I}_\epsilon(a+1,b-1)(t) - \mathcal{L}_\epsilon(a,b)(t)$$

which implies that the limit in (18) is given by:

$$\lim_{\epsilon \to 0}\left(\mathcal{I}_\epsilon(j,0)(t) - \sum_{i=0}^{j}\mathcal{L}_\epsilon(i,j-i)(t)\right)$$

We show that there exists a constant, depending only on ϕ and Ω, such that this quantity is bounded in absolute value by $const \cdot t^{\frac{m+1}{2}}$ for all $t \leq 1$. Since $|I_\epsilon\phi(t,r)| \leq \|\phi\|_{L^1(\Omega)}$ for all t, r and ϵ, $\mathcal{I}_\epsilon(j,0)(t)$ is going to be bounded above by a linear combinations, with coefficients depending only on ϕ and Ω, of terms of type:

$$\int_0^t \int_0^\infty r^{2i}\psi_{m-j-i}(t-\tau,r)\,dr\,d\tau$$

for $i = 0, \ldots, j$; each of these terms is a constant times t^{m-j+1}, and since $j \leq \frac{m+1}{2}$, $\lim_{\epsilon\to 0}\mathcal{I}_\epsilon(j,0)(t)$ is indeed $O(t^{\frac{m+1}{2}})$.

Now take a pair a, b of non-negative integers with $a + b = j \leq \frac{m+1}{2}$. By Lemma 15(ii), as $\lim_{\epsilon\to 0}\int_0^\infty \psi(r)\frac{\partial^{b-1}}{\partial \tau^{b-1}}I_\epsilon\phi(0,r)\,dr$ is a sum of terms of type $\frac{d^i\psi}{dr^i}(0)\int_{\partial\Omega}\phi_i$ for certain smooth functions ϕ_i and for $i = 0, \ldots, 2b-4$, we have, replacing ψ by $\frac{\partial^a}{\partial t^a}\psi_m(t,r)$, that $\lim_{\epsilon\to 0}\mathcal{L}_\epsilon(a,b)(t)$ is going to be a linear combinations of terms of type: $\frac{\partial^{2i}}{\partial r^{2i}}\frac{\partial^a}{\partial t^a}\psi_m(t,0)$ for $i = 0, \ldots, b-2$ and with coefficients depending only on ϕ and Ω. The i-th term is a constant times $t^{m-a-i-\frac{1}{2}}$; since $a + i \leq j - 2 \leq \frac{m-3}{2}$, it is in fact $O(t^{\frac{m+2}{2}})$. □

Proposition 20. *For all $m \in \mathbf{N}$, we have:*

$$I\phi(t,0) = \frac{1}{\sqrt{\pi}}\sum_{k=1}^{[\frac{m+1}{2}]}\int_{\partial\Omega} Z_k\phi \cdot t^{k-1/2} + \frac{1}{\sqrt{\pi}}\sum_{k=0}^{[\frac{m-1}{2}]}\int_0^t I\alpha_k\phi(\tau,0)(t-\tau)^{k-1/2}\,d\tau + O(t^{\frac{m+1}{2}})$$

where $Z_k = \sum_{j=0}^{k-1}\{k, j-1\}R_{k+j-1,j}$ *and* $\alpha_k = \sum_{j=0}^{k+1}\{k,j\}S_{k+j,j}$.

The proof is given in Appendix B.

Proof of the main Theorem. We can now prove that, for all $m \in \mathbf{N}$, and for all $\phi \in C_c^\infty(U)$, we have, as $t \to 0$:

$$I\phi(t,0) = \sum_{k=1}^{m}\beta_k(\phi)t^{k/2} + O(t^{\frac{m+1}{2}}) \tag{21}$$

and we prove the recursive formulas for the coefficients β_k.

The proof is by induction on m; we prove it for $m = 1$. By Duhamel principle applied to $I\phi(t, r)$:

$$I\phi(t,0) = -\frac{1}{\sqrt{\pi}} \int_0^t \frac{\partial}{\partial r} I\phi(\tau, 0)(t-\tau)^{-1/2}\, d\tau + \int_0^t \int_0^\infty e(t-\tau, r, 0) LI\phi(\tau, r)\, dr\, d\tau$$

Now $\frac{\partial}{\partial r} I\phi(\tau, 0) = -\int_{\partial\Omega} \phi$ for all $\tau > 0$; since $LI\phi(\tau, r) = \Lambda N\phi(\tau, r) - I\Delta\phi(\tau, r)$, and $|1 - u(\tau, x)| \leq 1$ for all τ, x, we see that:

$$|I\phi(t,0) - \frac{2}{\sqrt{\pi}} \int_{\partial\Omega} \phi \cdot t^{1/2}| \leq const \cdot t$$

where $const = \sup_{r\in(0,a)} |\int_{\rho^{-1}(r)} N\phi| + \|\Delta\phi\|_{L^1(\Omega)}$. Hence (21) holds for $m = 1$, and $\beta_1(\phi) = \frac{2}{\sqrt{\pi}} \int_{\partial\Omega} \phi$. Assume that (21) holds true for $m - 1$. Then, for all $k = 0, \ldots, [\frac{m-1}{2}]$:

$$I\alpha_k\phi(\tau, 0) = \sum_{j=1}^{m-1} \beta_j(\alpha_k\phi)\tau^{j/2} + O(\tau^{m/2})$$

Substituting in Proposition 20:

$$I\phi(t,0) = \frac{1}{\sqrt{\pi}} \sum_{k=1}^{[\frac{m+1}{2}]} \int_{\partial\Omega} Z_k\phi \cdot t^{k-1/2} + \frac{1}{\sqrt{\pi}} \sum_{k=0}^{[\frac{m-1}{2}]} \sum_{j=1}^{m-1} \frac{\Gamma(\frac{j}{2}+1)\Gamma(k+\frac{1}{2})}{\Gamma(k+\frac{j+3}{2})} \beta_j(\alpha_k\phi) t^{k+\frac{j+1}{2}} + O(t^{\frac{m+1}{2}})$$

We look at the coefficient of $t^{m/2}$ in the right-hand side of the above expression. If $m = 2n$ is even, then there is no contribution from the first sum, and the index j in the second sum must be odd, say $j = 2i - 1$, with $i = 1, \ldots, n$. Then $k = n - i$, and we get:

$$\beta_{2n}(\phi) = \frac{1}{\sqrt{\pi}} \sum_{i=1}^{n} \beta_{2i-1}(\alpha_{n-i}\phi) \frac{\Gamma(i+\frac{1}{2})\Gamma(n-i+\frac{1}{2})}{\Gamma(n+1)}$$

If $m = 2n + 1$ is odd, then j must be even, say $j = 2i$, with $i = 1, \ldots, n$, and we get:

$$\beta_{2n+1}(\phi) = \frac{1}{\sqrt{\pi}} \int_{\partial\Omega} Z_{n+1}\phi + \frac{1}{\sqrt{\pi}} \sum_{i=1}^{n} \beta_{2i}(\alpha_{n-i}\phi) \frac{\Gamma(i+1)\Gamma(n-i+\frac{1}{2})}{\Gamma(n+\frac{3}{2})}$$

The theorem follows for the initial data ϕ supported in the strip U, and then, as observed at the beginning of the section, for all $\phi \in C^\infty(\bar{\Omega})$. □

We now examine some consequences of the main theorem, in some special cases. We say that a function ϕ on Ω is *radial* (near $\partial\Omega$) if, on a neighborhood U of $\partial\Omega$, it depends only on the distance from the boundary; in other words, if $\phi(x) = f(\rho(x))$ for a function f on $[0, a)$, for some $a > 0$. If we now assume that $\Delta\rho$ itself is radial (in geometric terms, all parallel submanifolds which are close to the boundary have constant mean curvature), then the operators N and Δ take radial functions to radial functions. In fact, if r is the distance from the boundary, and if ϕ is a radial function (which we write, by a slight abuse of language, as $\phi(r)$), then:

$$\begin{aligned} N\phi(r) &= 2\phi'(r) - \phi(r)\Delta\rho(r) \\ \Delta\phi(r) &= -\phi''(r) + \phi'(r)\Delta\rho(r) \end{aligned} \tag{22}$$

In [4] it is proved that, for the upper hemisphere of a sphere, we have $\beta_{2n}(1) = 0$ for all $n \geq 1$. We can prove the following more general fact:

Theorem 23.

Assume that the domain Ω is such that $\Delta\rho(r)$ is an odd radial function on a neighborhood U of $\partial\Omega$ (in particular, we assume that $\partial\Omega$ is minimal). If the initial data $\phi(r)$ is an even radial function on U, then $\beta_{2n}(\phi) = 0$ for all $n \geq 1$.

Proof. We know that $\beta_{2n}(\phi)$ is given by integration over $\partial\Omega$ of $D_{2n}\phi$, where the operator D_{2n} is a polynomial of degree $2n-1$ in N and Δ. Since $D_{2n}\phi$ is a radial function, we have:

$$\beta_{2n}(\phi) = vol(\partial\Omega) \cdot D_{2n}\phi(0)$$

Observe that, under our assumptions, N takes even functions to odd functions (and viceversa) and that Δ preserves parity. Since D_{2n} has odd degree, it must take even functions to odd functions. Hence $D_{2n}\phi$ is odd, which implies that $D_{2n}\phi(0) = 0$. □

The theorem implies the above mentioned result for the upper hemisphere of the unit sphere S^m, because in that case $\Delta\rho(r) = (m-1)\tan r$ for $r < \frac{\pi}{2}$.

Finally, we verify our formulas for the unit ball in $\mathbf{R}^m$. Since $\Delta\rho(r) = \frac{m-1}{1-r}$, using equations (22), and our recursive formulas, one can easily recover the coefficients $\beta_1(1), \ldots, \beta_7(1)$ as computed in [4] (Theorem 4.2) by using Bessel's functions, and we find:

$$\beta_8(1) = \frac{\pi^{m/2}}{3072\Gamma(\frac{m}{2})}(m-1)(m-3)(m^4 + 15m^3 - 399m^2 + 1961m - 2298)$$

Moreover, since for a ball (or an annulus) in $\mathbf{R}^3$, $N\Delta\rho(r) = \Delta^2\rho(r) = 0$ for all r, we immediately have in that case: $\beta_k(1) = 0$ for all $k \geq 3$ (this fact was already observed in [4] and [8]).

Appendix A

In this appendix, we prove:

Proposition 6. *Let $\phi, \phi' \in C^\infty(\bar{\Omega})$. If $\phi = \phi'$ on a neighborhood U of $\partial\Omega$, then $\beta_k(\phi) = \beta_k(\phi')$ for all $k \geq 1$.*

Proof. For a domain in euclidean space, the proof is an immediate consequence of the so-called *principle of not feeling the boundary* , to the effect that $|1 - u(t,x)|$ is bounded by an exponentially decreasing function of t, as $t \to 0$, uniformly on each compact subset of Ω: in fact, by Levy's maximal inequality:

$$\begin{aligned} |1 - u(t,x)| &\leq 2\int_{\|y\| \geq \rho(x)} \frac{1}{(4\pi t)^{n/2}} e^{-\|y\|^2/4t}\, dy \\ &\leq 2ne^{-\rho(x)^2/4nt} \end{aligned}$$

for all $x \in \Omega$, and for all $t > 0$. Therefore, since $\phi - \phi'$ is supported on $\Omega(a)$, for some $a > 0$:

$$|\int_\Omega (1 - u(t,x))(\phi(x) - \phi'(x))\, dx| \leq 2n \cdot \sup_\Omega |\phi - \phi'| \cdot e^{-a^2/4nt}$$

and this implies that $\beta_k(\phi - \phi') = 0$ for all $k \geq 1$.

In general, let us assume that $\phi - \phi'$ is supported on $\Omega(2a)$ for some $a \in (0, R_{inj})$. We are going to show that, for each $m \in \mathbf{N}$, there are constants C_m and $T_m > 0$ depending only on Ω and a such that:

$$|1 - u(t,x)| \leq C_m t^m \tag{A.1}$$

for all $x \in \Omega(2a)$, and for all $t \leq T_m$. This clearly implies that $\beta_k(\phi - \phi') = 0$ for all $k \geq 1$. A.1 may be regarded as the principle of not feeling the boundary for Riemannian manifolds.

Then fix $x \in \Omega(2a)$, and let, for $r \geq 0$:

$$f(t,r) = \int_{\Omega(r)} k(t,x,y)\,dy$$

Note that: $f(t,0) = u(t,x)$. The function $f(t,r)$ is smooth on $(0,\infty) \times [0,a)$ and satisfies the following heat equation on $(0,a)$:

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\partial}{\partial t}\right) f(t,r) = -\int_{\rho^{-1}(r)} k(t,x,y)\Delta\rho(y)$$

Let $e_a(t,r,s)$ be the heat kernel of the interval $(0,a)$ satisfying Neumann boundary conditions at $r = 0$, and Dirichlet boundary conditions at $r = a$. By Duhamel principle, since $\dfrac{\partial f}{\partial r}(\tau,0) = 0$ for all $\tau > 0$:

$$u(t,x) = f(t,0) = \int_0^a e_a(t,r,0)\,dr + \int_0^t \frac{\partial e_a}{\partial r}(\tau,a,0) f(t-\tau,a)\,d\tau - \\ - \int_0^t \int_0^a e(t-\tau,r,0)\left(\int_{\rho^{-1}(r)} k(\tau,x,y)\Delta\rho(y)\,dy\right) dr\,d\tau$$

Now $|f(t,a)| \leq u(t,x) \leq 1$ for all t; moreover, if $v(t,r)$ denotes the solution of the heat equation on $(-a,a)$ satisfying $v(t,\pm a) = 1$ for all t, and $v(0,r) = 0$ for all r, then:

$$1 - \int_0^a e_a(t,r,0)\,dr = -\int_0^t \frac{\partial e_a}{\partial r}(\tau,a,0)\,d\tau = v(t,0)$$

Putting all these things together, we see that:

$$|1 - u(t,x)| \leq 2v(t,0) + \int_0^t \int_0^a e_a(t-\tau,r,0)\left(\int_{\rho^{-1}(r)} k(\tau,x,y)|\Delta\rho(y)|\,dy\right) dr\,d\tau \tag{A.2}$$

Both terms on the right are $O(t^m)$ for all m, uniformly in $x \in \Omega(2a)$. In fact: $v(t,0) \leq 2e^{-a^2/4t}$; by an estimate of Li and Yau (see [13]), there exist positive constants C and b, depending only on a lower bound of the Ricci curvature on a ball containing Ω, and on the dimension n of Ω, such that, for all $t > 0$:

$$k(t,x,y) \leq Ct^{-n/2} e^{-\frac{d(x,y)^2}{5t} + bt}$$

Since $\int_{\rho^{-1}(r)} |\Delta\rho|$ is bounded for $r \in (0,a)$, and since $d(x,y) > a$, we conclude that the second term in (A.2) is bounded above by a constant times $\displaystyle\int_0^t \tau^{-n/2} e^{-\frac{a^2}{5\tau} + b\tau}\,d\tau$, for all $x \in \Omega(2a)$. This proves (A.1) and the proposition. ☐

Appendix B

In this appendix, we prove Lemma B.9 and Lemma B.10 which, taken together with Lemma 17, will imply Proposition 20. We will make use of the following identities, which can be verified by differentiating $L^k I$ with respect to r in Lemma 12(iii):

$$\begin{cases} R_{ki} = Q_{ki} - NP_{ki} \\ S_{ki} = \Delta P_{ki} + P_{k,i-1} \end{cases} \tag{B.1}$$

The second relation implies, together with Lemma 15(iv):

$$\text{(B.2)} \qquad \sum_{i=1}^{p} \frac{\partial^i}{\partial t^i} I_\epsilon S_{ki}\phi(0,0) = \int_{\rho^{-1}(\epsilon)} \frac{\partial}{\partial \nu} P_{k0}\phi + (-1)^p \int_{\rho^{-1}(\epsilon)} \frac{\partial}{\partial \nu} \Delta^p P_{kp}\phi$$

The next lemma is a description of the distribution $L^k I\phi(0,r)$, and is needed in the proof of Lemma B.10. Since we will need to test $L^k I\phi(0,r)$ only on the function $r \mapsto e(t,r,0)$, we restrict to even test functions.

Lemma B.3. *Let $\psi \in C^\infty([0,\infty))$ be even at $r = 0$: $\psi^{(2i+1)}(0) = 0$ for all i. Then there are numbers $A_{ki} = A_{ki}(\phi)$ such that:*

$$\text{(i)} \qquad \int_0^\infty \psi(r) L^k I\phi(0,r)\, dr = \sum_{i=0}^{k} A_{ki}\psi^{(2i)}(0)$$

The numbers A_{ki} satisfy:

$$\text{(ii)} \qquad A_{k+j,j} = \sum_{i=j}^{k-2} \binom{i}{j} \int_{\partial\Omega} (R_{k+i,i+1} + \frac{\partial}{\partial \nu} P_{k+i,i+1})\phi$$

Proof of (i). From the formula:

$$\Delta(\psi \circ \rho) = -\psi^{(2)} \circ \rho + (\psi^{(1)} \circ \rho)\Delta\rho$$

one derives the formula:

$$\Delta(\phi(\psi \circ \rho)) = -(\psi^{(2)} \circ \rho)\phi - (\psi^{(1)} \circ \rho)N\phi + (\psi \circ \rho)\Delta\phi$$

hence, by induction, one shows that there exist operators V_{ij} on $C_c^\infty(U)$ such that:

$$\Delta^j(\phi(\psi \circ \rho)) = \sum_{i=0}^{2j} (\psi^{(2i)} \circ \rho) V_{ij}\phi$$

Since $\int_{\Omega(\epsilon)} \Delta^j(\phi(\psi \circ \rho)) = \int_{\rho^{-1}(\epsilon)} \frac{\partial}{\partial \nu} \Delta^{j-1}(\phi(\psi \circ \rho))$ we have, from Lemma 15, and letting $\epsilon \to 0$, that $L^k I\phi(0,r)$ is indeed a linear combination of the Dirac distribution at $r = 0$ and its derivatives.

Proof of (ii).

For $p \geq 0$, define the operators:

$$L^{k,p} I_\epsilon = \sum_{j=0}^{\infty} \frac{\partial^j}{\partial t^j} (\Lambda_\epsilon P_{k,p+j} + I_\epsilon Q_{k,p+j})$$

$$L^{k,p} \Lambda_\epsilon = \sum_{j=0}^{\infty} \frac{\partial^j}{\partial t^j} (\Lambda_\epsilon R_{k,p+j} + I_\epsilon S_{k,p+j})$$

and set: $L^{k,p} I\phi(0,r) = \lim_{\epsilon \to 0} L^{k,p} I_\epsilon\phi(0,r)$ in the sense of distributions. Then there are numbers A_{ki}^p such that:

$$\text{(B.4)} \qquad \int_0^\infty \psi(r) L^{k,p} I\phi(0,r)\, dr = \sum_{i=0}^{\infty} A_{ki}^p \psi^{(2i)}(0)$$

and: $A^p_{ki} = \dfrac{1}{(2i)!}\int_0^\infty r^{2i} L^{k,p} I\phi(0,r)\,dr$.

By using (B.1) and (14) one verifies easily that:

$$\text{(B.5)} \qquad \begin{aligned} L(L^{k,p}I_\epsilon) &= L^{k+1,p}I_\epsilon - I_\epsilon N P_{k,p-1} \\ \frac{\partial}{\partial r}L^{k,p}I_\epsilon &= -L^{k,p}\Lambda_\epsilon + I_\epsilon P_{k,p-1} \end{aligned}$$

Since $I_\epsilon\phi(0,r)$ and $\Lambda_\epsilon\phi(0,r)$ both vanish as $\epsilon \to 0$, we see that, integrating by parts:

$$\text{(B.6)} \quad \int_0^\infty \psi(r)L^{k+1,p}I\phi(0,r)\,dr = -\psi(0)L^{k,p}\Lambda\phi(0,0) - \int_0^\infty \psi^{(2)}(r)L^{k,p}I\phi(0,r)\,dr + \int_0^\infty \psi(r)L^{k,p-1}I\phi(0,r)\,dr$$

By (B.2), and Lemma 15:

$$L^{k,p}\Lambda\phi(0,0) = \int_{\partial\Omega}\left(R_{kp} + \frac{\partial}{\partial\nu}P_{kp}\right)\phi$$

We apply (B.6) to $\psi(r) = \dfrac{1}{(2i)!}r^{2i}$, and obtain the relations:

$$\text{(B.7)} \qquad \begin{cases} A^{p-1}_{k0} = A^p_{k+1,0} + \displaystyle\int_{\partial\Omega}\left(R_{kp} + \frac{\partial}{\partial\nu}P_{kp}\right)\phi \\ A^{p-1}_{ki} = A^p_{k+1,i} + A^p_{k,i-1} \qquad \text{if} \quad i \geq 1 \end{cases}$$

From (B.7), one proves that, for all p, k, j:

$$\text{(B.8)} \qquad A^p_{k+p+j,j} = \sum_{i=j}^{\infty}\int_{\partial\Omega}\binom{i}{j}\left(R_{k+p+i,p+i+1} + \frac{\partial}{\partial\nu}P_{k+p+i,p+i+1}\right)\phi$$

In fact, fix k, j; then $A^p_{k+p+j,j} = 0$ for $p = k$ (in fact, for $p \geq k$). Hence (B.8) holds for $p = k$, since $R_{2k+i,k+i+1} = P_{2k+i,k+i+1} = 0$ for all $i \geq 0$. Assuming (B.8) true for p, one verifies it for $p-1$ using relations (B.7). (B.8) then follows by induction. Taking $p = 0$ we obtain (ii). The upper limits in the sums (i) and (ii) follow from the last part of Lemma 12. $\square$

Lemma B.9. *Let $Z^{(m)}(t)$ be as in Lemma 17. Then:*

$$Z^{(m)}(t) = \frac{1}{\sqrt{\pi}}\sum_{k=1}^{[\frac{m+1}{2}]}\sum_{j=0}^{k-2}\int_{\partial\Omega}\{k,j\}\left(R_{k+j,j+1} + \frac{\partial}{\partial\nu}P_{k+j,j+1}\right)\phi \cdot t^{k-1/2} + O(t^{\frac{m+1}{2}})$$

Proof. Apply Lemma B.3 to $\psi(r) = e(t,r,0)$; since $\psi^{(2i)}(0) = \dfrac{(-1)^i}{\pi}\Gamma(i+\frac{1}{2})t^{-i-1/2}$, we obtain, setting $j = k-i$:

$$Z^{(m)}(t) = \frac{1}{\pi}\sum_{k=0}^{m}\sum_{j=0}^{k}\frac{(-1)^{k-j}}{k!}\Gamma(k-j+1/2)A_{k,k-j}t^{j-1/2}$$

Switching the two sums, and setting $i = k-j$, this can be re-written in the following form:

$$Z^{(m)}(t) = \frac{1}{\pi}\sum_{j=0}^{[\frac{m+1}{2}]}\tilde{Z}_j t^{j-1/2} + O(t^{\frac{m+1}{2}})$$

where:

$$\tilde{Z}_j = \sum_{i=0}^{j-1} \frac{(-1)^i}{(i+j)!} \Gamma(i+1/2) A_{i+j,i}$$

Taking into account Lemma B.3(ii) and switching the sums:

$$\tilde{Z}_j = \sum_{l=0}^{j-2} \left(\sum_{i=0}^{l} \frac{(-1)^i}{(i+j)!} \Gamma(i+\frac{1}{2}) \binom{l}{i} \right) \int_{\partial\Omega} (R_{j+l,l+1} + \frac{\partial}{\partial \nu} P_{j+l,l+1}) \phi$$

Now:

$$\begin{aligned} \sum_{i=0}^{l} \frac{(-1)^i}{(i+j)!} \Gamma(i+1/2) \binom{l}{i} &= \frac{1}{\Gamma(j+1/2)} \int_0^1 (1-\tau)^l \tau^{-1/2} (1-\tau)^{j-1/2} \, d\tau \\ &= \sqrt{\pi} \{j, l\} \end{aligned}$$

Substituting, we get the Lemma. □

Lemma B.10. *Let $B^{(m)}(t)$ be as in Lemma 17. Then:*

$$\begin{aligned} B^{(m)}(t) = \sum_{k=1}^{[\frac{m+1}{2}]} \int_{\partial\Omega} \{k,-1\} R_{k-1,0} \phi \cdot t^{k-1/2} - \sum_{k=1}^{[\frac{m+1}{2}]} \sum_{j=0}^{k-2} \int_{\partial\Omega} \{k, j\} \frac{\partial}{\partial \nu} P_{k+j,j+1} \phi \cdot t^{k-1/2} \\ + \sum_{k=1}^{[\frac{m+1}{2}]} \int_0^t I \alpha_k \phi(\tau, 0) (t-\tau)^{k-1/2} \, d\tau + O(t^{\frac{m+1}{2}}) \end{aligned}$$

Proof. By Lemma 12, $B^{(m)}(t)$ is the limit, as $\epsilon \to 0$, of $B_{1,\epsilon}^{(m)}(t) + B_{2,\epsilon}^{(m)}(t)$, where:

$$B_{1,\epsilon}^{(m)}(t) = \sum_{k=0}^{m} \sum_{j=0}^{k} \frac{1}{k!} \int_0^t \frac{\partial^j}{\partial \tau^j} \Lambda_\epsilon R_{kj} \phi(\tau, 0) (t-\tau)^{k-1/2} \, d\tau$$

$$B_{2,\epsilon}^{(m)}(t) = \sum_{k=0}^{m} \sum_{j=0}^{k} \frac{1}{k!} \int_0^t \frac{\partial^j}{\partial \tau^j} I_\epsilon S_{kj} \phi(\tau, 0) (t-\tau)^{k-1/2} \, d\tau$$

Because of the Dirichlet condition on u_ϵ, we have, for all ϵ:

$$\frac{\partial^j}{\partial \tau^j} \Lambda_\epsilon R_{kj} \phi(\tau, 0) = \begin{cases} 0 & \text{for all} \quad j \geq 1 \\ \int_{\partial\Omega} R_{k0} \phi & \text{if} \quad j = 0 \end{cases}$$

Hence:

$$\begin{aligned} B_{1,\epsilon}^{(m)}(t) &= \sum_{k=0}^{m} \int_{\partial\Omega} \frac{2}{k!(2k+1)} R_{k0} \phi \cdot t^{k+1/2} \\ &= \sum_{k=1}^{[\frac{m+1}{2}]} \int_{\partial\Omega} \{k,-1\} R_{k-1,0} \phi \cdot t^{k-1/2} + O(t^{\frac{m+1}{2}}) \end{aligned} \tag{B.11}$$

To deal with $B_{2,\epsilon}^{(m)}(t)$, we use Laplace transform with respect to t, and let: $\bar{f}(s) = \int_0^\infty e^{-st} f(t) \, dt$.

Laplace transform takes convolutions into products, $\overline{t^x} = \Gamma(x+1)s^{-x-1}$, and:

$$\overline{\frac{d^j f}{dt^j}}(s) = s^j \bar{f}(s) - \sum_{i=1}^{j} s^{i-1} \frac{d^{j-i} f}{dt^{j-i}}(0) \tag{B.12}$$

For the Laplace transform of $B_{2,\epsilon}^{(m)}(t)$ we then have:

$$\bar{B}_{2,\epsilon}^{(m)}(s) = \sum_{k=0}^{m} \sum_{j=0}^{k} \frac{\Gamma(k+\frac{1}{2})}{k!} \overline{I_\epsilon S_{kj} \phi}(s,0) s^{j-k-1/2} - \sum_{k=1}^{m} \sum_{j=1}^{k} \sum_{i=1}^{j} \frac{\Gamma(k+\frac{1}{2})}{k!} \frac{\partial^{j-i}}{\partial \tau^{j-i}} I_\epsilon S_{kj} \phi(0,0) s^{i-k-3/2} \tag{B.13}$$

Since $\sum_{k=0}^{m} \sum_{j=0}^{k} a_{kj} = \sum_{k=0}^{m} \sum_{j=0}^{m-k} a_{k+j,j}$, the inverse Laplace tranform of the first term of (B.13) is:

$$\sum_{k=0}^{m} \int_0^t I_\epsilon \alpha_k^{(m)} \phi(\tau,0)(t-\tau)^{k-1/2}\, d\tau \tag{B.14}$$

where $\alpha_k^{(m)}$ is the operator: $\alpha_k^{(m)} = \sum_{j=0}^{m-k} \{k,j\} S_{k+j,j}$

Since $|I_\epsilon \psi(\tau,0)| \leq Const$, for all τ, and all ϵ, (B.14) can be written as:

$$\sum_{k=0}^{[\frac{m-1}{2}]} \int_0^t I_\epsilon \alpha_k^{(m)} \phi(\tau,0)(t-\tau)^{k-1/2}\, d\tau + O(t^{\frac{m+1}{2}}) \tag{B.15}$$

If $k \leq [\frac{m-1}{2}]$, then $m-k \geq k+1$; since $S_{k+j,j} = 0$ for $j > k+1$, we conclude that the inverse Laplace transform of the first term in (B.13) is:

$$\sum_{k=0}^{[\frac{m-1}{2}]} \int_0^t I_\epsilon \alpha_k \phi(\tau,0)(t-\tau)^{k-1/2}\, d\tau + O(t^{\frac{m+1}{2}}) \tag{B.16}$$

where $\alpha_k = \sum_{j=0}^{k+1} \{k,j\} S_{k+j,j}$.

We now examine the second term in (B.13). We re-arrange the sum in the following way:

$$\sum_{k=1}^{m} \sum_{j=1}^{k} \sum_{i=1}^{j} a_{kji} = \sum_{k=1}^{m} \sum_{j=0}^{m-k} \sum_{i=0}^{k-1} a_{k+j,j+i+1,j+1} \tag{B.17}$$

(the steps are: switch the last two sums and change j to $l = j - i$; get: $\sum_{k=1}^{m} \sum_{j=1}^{k} \sum_{l=0}^{k-i} a_{k,i+l,i}$; switch the first two sums and change k to $p = k - i$; get: $\sum_{i=1}^{m} \sum_{p=0}^{m-i} \sum_{l=0}^{p} a_{p+i,i+l,i}$; now change p to $q = p+1$, i to $n = i-1$ and then switch the first two sums; get: $\sum_{q=1}^{m} \sum_{n=0}^{m-q} \sum_{l=0}^{p-1} a_{q+n,n+l+1,n+1}$ After renaming, we obtain B.17).

The inverse Laplace transform of the second term in (B.13) can then be written as:

$$-\sum_{k=1}^{m} \sum_{j=0}^{m-k} \frac{\Gamma(k+j+1/2)}{(k+j)!\Gamma(k+1/2)} \sum_{i=0}^{k-1} \frac{\partial^i}{\partial \tau^i} I_\epsilon S_{k+j,j+i+1} \phi(0,0) t^{k-1/2} \tag{B.18}$$

By B.2, since $P_{k+j,k+j} = 0$:

$$\sum_{i=0}^{k-1} \frac{\partial^i}{\partial \tau^i} I_\epsilon S_{k+j,j+i+1}\phi(0,0) = I_\epsilon S_{k+j,j+1}\phi(0,0) + \int_{\rho^{-1}(\epsilon)} \frac{\partial}{\partial \nu} P_{k+j,j+1}\phi$$

As $\epsilon \to 0$, $I_\epsilon S_{k+j,j+1}\phi(0,0) \to 0$. Hence (B.18) becomes:

$$-\sum_{k=1}^{m} \sum_{j=0}^{m-k} \int_{\rho^{-1}(\epsilon)} \frac{\partial}{\partial \nu} \left(\{k,j\} P_{k+j,j+1}\phi\right) t^{k-1/2} + O(\epsilon)$$

Once again, modulo terms of order $t^{\frac{m+1}{2}}$ and higher, we can restrict k to the range $k = 0, \ldots, [\frac{m+1}{2}]$. Since $P_{k+j,j+1} = 0$ for $j > k-3$, the inverse Laplace transform of the second term of (B.13) can be re-written:

$$\text{(B.19)} \qquad -\sum_{k=1}^{[\frac{m+1}{2}]} \sum_{j=0}^{k-2} \int_{\partial\Omega} \frac{\partial}{\partial \nu} \left(\{k,j\} P_{k+j,j+1}\phi\right) t^{k-1/2} + O(t^{\frac{m+1}{2}}) + O(\epsilon)$$

Taking into account (B.11),(B.13),(B.16) and (B.19), and passing to the limit as $\epsilon \to 0$, we obtain the lemma. □

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