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Short-Time Heat Content Asymptotics via the Wave and Eikonal Equations

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Abstract

In this short paper, we derive an alternative proof for some known (van den Berg & Gilkey 2015) short-time asymptotics of the heat content in a compact full-dimensional submanifolds S with smooth boundary. This includes formulae like

$$\int_S \exp(t\Delta)(f\mathbb{1}_S)\,\mathrm{d}V = \int_S f\,\mathrm{d}V - \sqrt{\frac{t}{\pi}}\int_{\partial S} f\,\mathrm{d}A + o(\sqrt{t}), \quad t \to 0^+,$$

and explicit expressions for similar expansions involving other powers of $\sqrt{t}$. By the same method, we also obtain short-time asymptotics of $\int_S \exp(t^m\Delta^m)(f\mathbb{1}_S)\,\mathrm{d}V$, $m \in \mathbb{N}$, and more generally for one-parameter families of operators $t \mapsto k(\sqrt{-t\Delta})$ defined by an even Schwartz function k.

Keywords Heat equation · Heat content · Riemannian manifolds · Geometrical optics

1 Introduction

Let (M, g) be a complete, boundaryless,[1] oriented Riemannian manifold with Laplace–Beltrami operator Δ, and volume $\mathrm{d}V$. On a codimension-1 submanifold of M, we write $\mathrm{d}A$ for the induced surface (hyper)-area form. The *heat semi-group* $T_t := \exp(t\Delta)$ acting on $L^2(M, \mathrm{d}V)$ is well defined (Δ is essentially self-adjoint on $C_c^\infty(M)$ [2]) and its behaviour as $t \to 0^+$ has been extensively investigated in the literature. Specifically, for a set $S \subset M$, the *heat content* of the form

[1] We assume that M has no boundary for the sake of simplicity, and the method presented here can be adapted to more general manifolds with boundary provided that S is compactly contained in the interior of M. If this is not the case, such as in the classical heat content setting as in [13], it should be possible to obtain similar results by modifying the geometrical optics construction used.

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$\Omega_{S,f}(t) := \int_S T_t(f\mathbb{1}_S)\,\mathrm{d}V,\ f \in C^\infty(M)$, has recently received much attention; see, for instance, [7,11,12] and the references therein.

Let us briefly recall some known results. On $\mathbb{R}^n$, sets S of *finite perimeter* $P(S)$ are characterized by [7, Thm. 3.3]

$$\lim_{t\to 0^+}\sqrt{\frac{\pi}{t}}\Big(\Omega_{S,\mathbb{1}_M}(0)-\Omega_{S,\mathbb{1}_M}(t)\Big)=P(S). \tag{1}$$

Extensions of this idea to abstract metric spaces are given in [6]. In the setting of compact manifolds M (or $M = \mathbb{R}^n$) and S a full-dimensional submanifold with smooth boundary ∂S, the authors of [12] show that

$$\Omega_{S,f}(t)=\sum_{j=0}^{\infty}\beta_j t^{\frac{j}{2}}, \quad t\to 0^+, \tag{2}$$

where the coefficients β_j depend on S, f and the geometry of M. The setting of [12] is more general, amongst other things it includes f which have singularities. Some of the coefficients obtained in [12, corollary 1.7] are

$$\beta_0=\int_S f\,\mathrm{d}V, \quad \beta_1=-\frac{1}{\sqrt{\pi}}\int_{\partial S} f\,\mathrm{d}A, \quad \beta_2=\frac{1}{2}\int_S \Delta f\,\mathrm{d}V.$$

Extensions to some non-compact manifolds M and certain non-compact S are in [11].

Both Eqs. (1) and (2) are proven with significant technical effort, yielding strong results. For example, in [7], explicit knowledge of the fundamental solution of the heat equation is used to obtain Eq. (1) for $C^{1,1}$-smooth ∂S, after which geometric measure theory is used. Similarly, [12] requires pseudo-differential calculus and invariance theory.

Our aim is to show that slightly weaker results can be obtained by considerably lower technical effort. In contrast to [7], we treat only compact S with smooth boundary, and do not allow f to have singularities like [12] does. On the other hand, we put no further restrictions than completeness on M. The proof presented here is simple, comparatively short, and provides an alternative differential geometric/functional analytic point of view to questions regarding heat content. Moreover, this approach is readily extended to some other PDEs including the semi-group generated by Δ^m. Observe that $T(t) = k(\sqrt{-t\Delta})$ with $k(x) = \exp(-x^2)$. We allow k to be an arbitrary even Schwarz function, with $\Omega_{S,f}(t) = \int_S k(\sqrt{-t\Delta})(f\mathbb{1}_S)\,\mathrm{d}V$ and will prove:

Theorem 1 *Let M be a complete Riemannian manifold with Laplace–Beltrami operator Δ, Riemannian volume $\mathrm{d}V$ and induced (hyper) area form $\mathrm{d}A$. Let $S \subset M$ be a compact full-dimensional submanifold with smooth boundary. For $f \in C^\infty(M)$ and $N \in \mathbb{N}$,*

$$\Omega_{S,f}(t)=\sum_{j=0}^{N}\beta_j t^{\frac{j}{2}}+o(t^{\frac{N}{2}}), \quad t\to 0^+,$$

for constants $(\beta_j)_{j=0}^N$ described further in the next theorem.

With the jth derivative $k^{(j)}$ (for $j \in \mathbb{N}_0$), let $r_j := (-1)^{j/2} k^{(j)}(0)$ for j even and $r_j := (-1)^{(j-1)/2} \int_0^\infty \frac{2k^j(s)}{-\pi s}\, \mathrm{d}s$ for j odd. Let φ locally be the signed distance function (see also [8, Sect. 3.2.2]) to ∂S with $S = \varphi^{-1}([0, \infty))$, and denote by ∇ and $\cdot$ the gradient and (metric) inner product, respectively. The vector field $\nu := -\nabla\varphi$ is outer unit normal at ∂S.

Theorem 2 *The coefficients of Theorem 1 satisfy $\beta_0 = r_0 \int_S f\, \mathrm{d}V$ and $\beta_1 = -\frac{1}{2} r_1 \int_{\partial S} f\, \mathrm{d}A$. For even $j \in \mathbb{N}_{\geq 2}$,*

$$\beta_j = \frac{r_j}{j!} \int_S \frac{1}{2} \Delta^{j/2} f\, \mathrm{d}V.$$

Moreover, given the Lie-derivative $\mathcal{L}_\nu$ with respect to ν,

$$\beta_3 = \frac{r_3}{2 \cdot 3!} \int_{\partial S} \mathcal{L}_\nu(-\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi) f - \frac{1}{2}\Delta f + \frac{1}{2}(-\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi)^2 f\, \mathrm{d}A,$$

similar expression can be found also for larger odd values of j (see Sect. 3).

The properties of the signed distance function φ may be used to express terms appearing in Theorem 2 using other quantities. For example, its Hessian $\nabla^2\varphi$ is the second fundamental form on the tangent space of ∂S [3, Chap. 3], and thus $\frac{1}{2}\Delta\varphi$ is the mean curvature.

Our approach to prove Theorems 1 and 2 is to combine 3 well-known facts:

(A) The short-time behaviour of the heat flow is related to the short-time behaviour of the wave equation (cf. [1]).

(B) The short-time behaviour of the wave equation with discontinuous initial data is related to the short-time behaviour of the eikonal equation (cf. 'geometrical optics' and the progressing wave expansion [10]).

(C) The short-time behaviour of the wave and eikonal equations with initial data $f\mathbb{1}_S$ is directly related to the geometry of M near ∂S.

Though points (A)-(C) are well known in the literature, they have (to the best of our knowledge) not been applied to the study of heat content so far.

A significant portion of (C) will rest on an application of the Reynolds transport theorem. Here, denote by Φ^s the time-s flow of the vector field $\nu = -\nabla\varphi$. For small s, the (half) tubular neighbourhood

$$S^{-s} := \{x \in M \setminus S : \mathrm{dist}(x, \partial S) \leq s\} \tag{3}$$

satisfies $S \cup S^{-s} = \Phi^s(S)$. For $a \in C^\infty((-\varepsilon, \varepsilon) \times M)$, by [5, Chap. V, Prop. 5.2],

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}s} \int_{S^{-s}} a(s, \cdot)\, \mathrm{d}V \bigg|_{s=0} &= \frac{\mathrm{d}}{\mathrm{d}s} \left(\int_{S^{-s} \cup S} a(s, \cdot)\, \mathrm{d}V - \int_S a(s, \cdot)\, \mathrm{d}V \right) \bigg|_{s=0} \\ &= \int_S \mathcal{L}_{\tilde{\nu}}[a(0, \cdot)\, \mathrm{d}V] = \int_{\partial S} a(0, \cdot)\, \mathrm{d}A. \end{aligned} \tag{4}$$

The last equation is a consequence of Cartan's magic formula and Stokes' theorem, where we use that $\mathrm{d}V(\nu, \cdot) = \mathrm{d}A(\cdot)$ on ∂S.

2 Proof for β_0, β_1

By Fourier theory (for non-Gaussian k, the formulae must be adapted),

$$k(t) = \exp(-t^2) = \int_0^\infty \hat{k}(s)\cos(ts)\,\mathrm{d}s \quad \text{with} \quad \hat{k}(s) := \frac{1}{\sqrt{\pi}}\exp\left(\frac{-s^2}{4}\right).$$

On the operator level, this yields the well-known formula [10, Sect. 6.2]

$$T_t = \exp(t\Delta) = \int_0^\infty \hat{k}(s)\cos(s\sqrt{-t\Delta})\,\mathrm{d}s. \tag{5}$$

The operator $W^s := \cos(s\sqrt{-\Delta})$ is the time-s solution operator for the wave equation with zero initial velocity, in particular $u(s,x) := (W^s f \mathbb{1}_S)(x)$ (weakly) satisfies $(\partial_t^2 - \Delta)u = 0$. Let $\langle \cdot, \cdot \rangle$ denote the $L^2(M, \mathrm{d}V)$ inner product. Using Eq. (5),

$$\langle T_t f \mathbb{1}_S, \mathbb{1}_S \rangle = \int_0^\infty \hat{k}(s)\langle W_{s\sqrt{t}} f \mathbb{1}_S, \mathbb{1}_S \rangle\,\mathrm{d}s.$$

Similar reasoning has been used to great effect in [1] to derive heat-kernel bounds by making use of the *finite propagation speed* of the wave equation. As in [1], finite propagation speed yields for $s \geq 0$ that $\langle W_s f \mathbb{1}_S, \mathbb{1}_{M\setminus S} \rangle = \langle W_s f \mathbb{1}_{S^s}, \mathbb{1}_{S^{-s}} \rangle$, where $S^s := (M \setminus S)^{-s}$ is defined like Eq. (3). Even if $\mathbb{1}_{M\setminus S} \notin L^2(M, \mathrm{d}V)$, we have just seen that the inner product $\langle W_s f \mathbb{1}_S, \mathbb{1}_{M\setminus S} \rangle$ is nevertheless well defined. In [1], it is further observed that $\| W_s \| \leq 1$. Using the Cauchy–Schwarz inequality and assuming $f = \mathbb{1}_M$, Eq. (4) yields

$$h(s) := \langle W_s f \mathbb{1}_{S^s}, \mathbb{1}_{S^{-s}} \rangle \leq \|\mathbb{1}_{S^s}\|_2 \|\mathbb{1}_{S^{-s}}\|_2 \leq s\int_{\partial S} \mathrm{d}A + o(s), \quad s \to 0^+. \tag{6}$$

In addition, $|\langle W_s f \mathbb{1}_S, \mathbb{1}_S \rangle| \leq \|f\mathbb{1}_S\|_2 \|\mathbb{1}_S\|_2$ for all $s \geq 0$, in particular as $s \to \infty$. We conclude with some calculations (cf. Lemma 3), that

$$\begin{aligned} \langle T_t \mathbb{1}_S, \mathbb{1}_S \rangle &= \int_0^\infty \hat{k}(s)\left(\langle W_{s\sqrt{t}} \mathbb{1}_S, \mathbb{1}_M \rangle - \langle W_{s\sqrt{t}} \mathbb{1}_S, \mathbb{1}_{M\setminus S} \rangle\right)\,\mathrm{d}s \\ &= \langle \mathbb{1}_S, \mathbb{1}_M \rangle - \int_0^\infty \hat{k}(s) h(s\sqrt{t})\,\mathrm{d}s \\ &\geq \int_S \mathrm{d}V - 2\sqrt{\frac{t}{\pi}}\int_{\partial S}\mathrm{d}A + o(\sqrt{t}), \qquad t \to 0^+. \end{aligned} \tag{7}$$

This is weaker than the desired estimate, and restricts to $f = \mathbb{1}_M$. The problem is that the estimates in Eq. (6) are too crude. To improve them, we instead approximate the solution u to the wave equation with geometrical optics, using the "progressing wave" construction described in [10, Sect. 6.6], some details of which we recall here. The basic idea is that u is in general discontinuous, with an outward—and an inward—moving discontinuity given by the zero level-set of functions φ^+ and φ^-, respectively. The functions $\varphi^\pm$ satisfy the eikonal equation $\partial_t\varphi = \pm|\nabla\varphi^\pm|$ with initial value $\varphi^\pm(0,\cdot) = \varphi(\cdot)$. Equivalently, using the (nonlinear) operator $Ew := (\partial_t w)^2 - |\nabla w|^2$, the functions $\varphi^\pm$ satisfy $E(\varphi^\pm) = 0$. Our analysis is greatly simplified by choosing the initial φ to (locally) be the signed distance function to ∂S. The eikonal equation is then $\partial_t\varphi^\pm = \pm|\nabla\varphi| = \pm|-\nu| = \pm 1$, i.e. $\varphi^\pm(x,t) = \varphi(x) \pm t$.

The progressing wave construction further makes use of two (locally existing and smooth) solutions $a_0^\pm$ to the first-order transport equations $\pm\partial_t a_0^\pm(t,\cdot) + \nu\cdot\nabla a_0^\pm(t,x) = \frac{1}{2}a_0^\pm\Delta\varphi^\pm$. Observe that with the Heaviside function $\theta\colon \mathbb{R}\to\mathbb{R}$, and $\Box := \partial_t^2 - \Delta$, the expression $\Box(a_0^\pm\theta(\varphi^\pm))$ is given by

$$(\theta''(\varphi^\pm)E\varphi^\pm + \Box\varphi^\pm\theta'(\varphi^\pm))a_0^\pm + 2\left(\partial_t a_0^\pm\partial_t\varphi^\pm - \nabla a_0^\pm\cdot\nabla\varphi^\pm\right)\theta'(\varphi^\pm) + \Box a_0^\pm\theta(\varphi^\pm).$$

The functions $\varphi^\pm$ and $a_0^\pm$ have been chosen so the above simplifies to

$$\begin{aligned}\Box(a_0^\pm\theta(\varphi^\pm)) &= 2\left(\pm\partial_t a_0^\pm + \nabla a_0^\pm\cdot\nu - \frac{1}{2}\Delta\varphi a_0^\pm\right)\theta'(\varphi^\pm) + \Box a_0^\pm\theta(\varphi^\pm)\\ &= \Box a_0^\pm\theta(\varphi^\pm).\end{aligned} \tag{8}$$

Thus $\Box(a_0^\pm\theta(\varphi^\pm))$ is as smooth as θ is. We use

$$\tilde{u}(t,x) := a_0^+(t,x)\theta(\varphi^+(t,x)) + a_0^-(t,x)\theta(\varphi^-(t,x))$$

as an approximation to the discontinuity of the solution u to the wave equation. To maintain consistency with the initial values of u, the initial values of the approximation $\tilde{u}$ are chosen to coincide with those of u at $t = 0$, this is achieved by setting $a_0^\pm(0,\cdot) = \frac{1}{2}f$ so that (at least formally) $\partial_t\tilde{u}(0,\cdot) = 0$ and also $\tilde{u}(0,\cdot) = \mathbb{1}_S f$.

The function $\tilde{u}$ approximates the discontinuous solution u of the wave equation well enough that the function $(s,x)\mapsto u(s,x) - \tilde{u}(s,x)$ is continuous on $[-T,T]\times M$, see [10, Sect. 6.6, eq. 6.35]. By construction, $\tilde{u}(0,\cdot) = u(0,\cdot)$. Hence $|(u(s,x) - \tilde{u}(s,x)| = o(1)$ as $s\to 0^+$, which implies

$$|\langle u(s,\cdot),\mathbb{1}_{S^{-s}}\rangle - \langle\tilde{u}(s,\cdot),\mathbb{1}_{S^{-s}}\rangle| = o(s) \quad s\to 0^+. \tag{9}$$

As $\nabla\varphi = -\nu$, for sufficiently small t the sets $\{x\in M : \varphi^+(t,x) = 0\}$ (resp. $\{x : \varphi^-(t,x) = 0\}$) are level sets of φ on the outside (resp. inside) of S (see also [10, Sect. 6.6]). By construction, $\theta(\varphi^-)$ vanishes outside of S for $t > 0$. Consequently, using Eq. (4), we see that as $s \to 0^+$,

$$\begin{aligned} \langle \tilde{u}(s,\cdot), \mathbb{1}_{S^{-s}} \rangle &= \int_{S^{-s}} a_0^+(s,x)\mathbb{1}_{\{\varphi^+(s,\cdot)\geq 0\}} + a_0^-(s,x)\mathbb{1}_{\{\varphi^-(s,x)\geq 0\}}\, \mathrm{d}V(x) \\ &= s\int_{\partial S} a_0^+(0,x)\,\mathrm{d}A(x) + o(s) = \frac{s}{2}\int_{\partial S} f\,\mathrm{d}A + o(s). \end{aligned} \tag{10}$$

Combining Eqs. (9) and (10),

$$h(s) = \langle W_s f \mathbb{1}_S, \mathbb{1}_{S^{-s}} \rangle = \langle u(s,\cdot), \mathbb{1}_{S^{-s}} \rangle = \frac{s}{2}\int_{\partial S} f\,\mathrm{d}A + o(s), \quad s \to 0^+.$$

Calculations along the lines of Lemma 3 and Eq. (7) yield

$$\langle T_t f \mathbb{1}_S, \mathbb{1}_S \rangle = \int_S f\,\mathrm{d}V - \sqrt{\frac{t}{\pi}}\int_{\partial S} f\,\mathrm{d}A + o(\sqrt{t}), \qquad t \to 0^+,$$

as claimed.

Lemma 3 *Let $j \in \mathbb{N}$ and $\gamma : \mathbb{R}_{\geq 0} \to \mathbb{R}$. Let $\gamma(s) = s^j + o(s^j)$ for $s \to 0$ and $\gamma(s) = O(1)$ for $s \to \infty$. Then for $t \to 0^+$,*

$$\int_0^\infty \gamma(s\sqrt{t})\hat{k}(s)\,\mathrm{d}s = t^{\frac{j}{2}} \begin{cases} (-1)^{\frac{j}{2}}\, k^{(j)}(0) & j \text{ even} \\ (-1)^{\frac{j-1}{2}} \int_0^\infty \frac{2\,k^{(j)}(s)}{-\pi s}\,\mathrm{d}s & j \text{ odd} \end{cases} + o\left(t^{\frac{j}{2}}\right). \tag{11}$$

With $k(s) = \exp(-s^2)$ and $h(s) = c_0 + c_1 s + c_2 s^2 + o(s^2)$, this implies

$$\int_0^\infty h(s\sqrt{t})\hat{k}(s)\,\mathrm{d}s = c_0 + \frac{2c_1}{\sqrt{\pi}}\sqrt{t} + 2c_2 t + o(t). \tag{12}$$

Proof For even j, we obtain Eq. (11) by the Fourier-transform formula for jth derivatives. If j is odd, we also need to multiply by the sign function in frequency space, and then use that the inverse Fourier-transform (unnormalized) of the sign function is given by the principal value p.v. $\left(\frac{2i}{x}\right)$ [10, Sect. 4], see also [9, Chap. 7]. Equation 11 holds more generally, e.g. if k is an even Schwarz function. Equation 12 may also be verified directly without Eq. (11). □

3 Proof for $\beta_2, \beta_3, \ldots$

We now turn to calculating β_j for $j \geq 2$. We use the Nth order progressing wave construction with sufficiently large $N \gg j$. For the sake of simplicity, we write $O(t^\infty)$ for quantities that can be made $O(t^k)$ for any $k \in \mathbb{N}$ by choosing sufficiently large N. As in the previous section, the construction is from [10, Sect. 6.6]. With

$\theta_0 := \theta$, and $\theta_i(t) := \int_{-\infty}^t \theta_{i-1}(s)\mathrm{d}s$ we write

$$\tilde{u}^{\pm}(t,x) := \sum_{i=0}^{N} a_i^{\pm}(t,x)\theta_i(\varphi^{\pm}(t,x)).$$

Here the functions $a_0^{\pm}$ are defined as before, and for $i \geq 1$ the ith order transport equations $\pm\partial_t a_i^{\pm} = -\nu \cdot \nabla a_i^{\pm} + \frac{1}{2}a_i^{\pm}\Delta\varphi^{\pm} - \frac{1}{2}\Box a_{i-1}^{\pm}$ define $a_i^{\pm}$ together with initial data $a_i^{\pm}(0,\cdot) = -\frac{1}{2}(\partial_t a_{i-1}^{+}(0,\cdot) + \partial_t a_{i-1}^{-}(0,\cdot))$. As in Eq. (8), one may verify that $\Box\tilde{u}^{\pm} = \Box a_i \theta_N(\varphi^{\pm})$. Writing $\tilde{u} = \tilde{u}^{+} + \tilde{u}^{-}$ and

$$u(t,x) = \tilde{u}^{+}(t,x) + \tilde{u}^{-}(t,x) + R_N(t,x),$$

the remainder satisfies $R_N \in C^{(N,1)}([-T,T]\times M)$ and $R_N(t,\cdot)$ vanishes at $t=0$, see [10, Sect. 6.6, eq. 6.35]. Moreover, R_N is supported on $\{(x,t) : \mathrm{dist}(x,S) \leq |t|\}$, all of this implies that, as $t \to 0^{+}$,

$$h(t) = \int_{M\setminus S} u(t,x)\,\mathrm{d}V(x) = \int_{M\setminus S} \tilde{u}^{+}(t,x)\,\mathrm{d}V(x) + O(t^{\infty}) \tag{13}$$

and moreover $h \in C^{\infty}([0,T])$. The structure of R_N implies that $\Box\tilde{u}^{+}(t,x) = O(t^{\infty})$ on $M \setminus S$, provided that this expression is interpreted in a sufficiently weak sense. Formally, therefore

$$\begin{aligned}\partial_t^2 \int_{M\setminus S} \tilde{u}^{+}(\cdot,t)\,\mathrm{d}V &= \int_{M\setminus S} \Delta\tilde{u}^{+}(\cdot,t)\,\mathrm{d}V + O(t^{\infty})\\ &= -\int_{\partial S} \nabla\tilde{u}^{+}(\cdot,t)\cdot\nu\,\mathrm{d}A + O(t^{\infty}),\end{aligned} \tag{14}$$

where the last step is the divergence theorem. One may verify Eq. (14) rigorously by either doing the above steps in the sense of distributions, or by a (somewhat tedious) manual computation. Combining this with Eq. (13),

$$h''(t) = -\int_{\partial S} \nabla\tilde{u}^{+}(\cdot,t)\cdot\nu\,\mathrm{d}A + O(t^{\infty}). \tag{15}$$

The quantity $h^{(j)}(0)$ may thus be seen to depend $\tilde{u}^{+}(0,\cdot)$ at ∂S, which in turn depends on $a_i^{\pm}$ at $t=0$. Defining $\mathbf{S}_i := a_i^{+} + a_i^{-}$ and $\mathbf{D}_i := a_i^{+} - a_i^{-}$ for $i = 0, 1, \ldots$, let L be the (spatial) differential operator defined for $w \in C^{\infty}(M)$ by $Lw := \frac{1}{2}\Delta\varphi w - \nu\cdot\nabla w$. For $i \in \mathbb{N}_0$, the transport equations imply

$$\partial_t\mathbf{S}_0 = L\mathbf{D}_0, \qquad \partial_t\mathbf{D}_0 = L\mathbf{S}_0, \tag{16}$$

$$\partial_t\mathbf{S}_{i+1} = L\mathbf{D}_{i+1} - \frac{1}{2}\Box\mathbf{D}_i, \qquad \partial_t\mathbf{D}_{i+1} = L\mathbf{S}_{i+1} - \frac{1}{2}\Box S_i \quad \text{for} \quad i \geq 0, \tag{17}$$

with initial values satisfying

$$a_0^+(0,\cdot) = \frac{1}{2}\mathbf{S}_0(0,\cdot) = \frac{1}{2}f(\cdot), \qquad \mathbf{D}_0(0,\cdot) = 0, \tag{18}$$

$$a_{i+1}^+(0,\cdot) = \frac{1}{2}\mathbf{D}_{i+1}(0,\cdot) = -\frac{1}{2}\partial_t\mathbf{S}_i(0,\cdot), \quad \mathbf{S}_{i+1}(0,\cdot) = 0. \tag{19}$$

Lemma 4 *For $i, n \in \mathbb{N}_0$ it holds that $\partial_t^{2n}\mathbf{D}_i(0,\cdot) = 0$ (note that as a consequence, also $a_{i+1}(0,\cdot)$, $L\mathbf{D}_i(0,\cdot)$, and $\Box^n\mathbf{D}_i(0,\cdot)$ are zero).*

Proof We will proceed by induction over i and use the identities Eqs. (16)–(19). For $i = 0$, $\mathbf{D}_0(0,\cdot) = 0$ is trivially satisfied. Moreover, $\partial_t^{2n}\mathbf{D}_0 = R^n\mathbf{D}_0$, which is zero at $t = 0$. For $i = 1$, observe that $a_1^+(0,\cdot) = -\frac{1}{2}\partial_t\mathbf{S}_0(0,\cdot) = -\frac{1}{2}L\mathbf{D}_0(0,\cdot) = 0$, and thus $\mathbf{D}_1(0,\cdot) = 0$. Likewise, $\partial_t^2\mathbf{D}_1 = \partial_t(L\mathbf{S}_1 - \frac{1}{2}\Box\mathbf{S}_0) = L(L\mathbf{D}_1 - \frac{1}{2}\Box\mathbf{D}_0) - \frac{1}{2}\Box L\mathbf{D}_0$. As the operator L commutes with ∂_t^2, this expression vanishes at $t = 0$. Induction over n proves the remainder of the statement for $i = 1$. For the general case, we assume the induction hypothesis for i and $i+1$ and start by noting that $\mathbf{D}_{i+2}(0,\cdot) = 2a_{i+2}^+(0,\cdot) = -\partial_t\mathbf{S}_{i+1}(0,\cdot) = -\big(L\mathbf{D}_{i+1}(0,\cdot) - \frac{1}{2}\Box\mathbf{D}_i(0,\cdot)\big) = 0$. Moreover, $\partial_t^2\mathbf{D}_{i+2} = \partial_t(L\mathbf{S}_{i+2} - \frac{1}{2}\Box\mathbf{S}_{i+1}) = L(L\mathbf{D}_{i+2} - \frac{1}{2}\Box\mathbf{D}_{i+1}) - \frac{1}{2}\Box\big(L\mathbf{D}_{i+1} - \frac{1}{2}\Box\mathbf{D}_i\big)$, which again vanishes at $t = 0$; the case $n > 1$ may again be proven by induction over n. □

Corollary 5 *For even $j \in \mathbb{N}_{\geq 2}$, the jth derivative of h satisfies*

$$h^{(j)}(0) = -\frac{1}{2}\int_S \Delta^{j/2} f \,\mathrm{d}V.$$

Proof Lemma 4 shows that for $i \geq 1$, $a_i^+(0,x) = 0$. Together with Eq. (15), thus $h''(0) = -\int_{\partial S}\nabla a_0^+(0,\cdot)\cdot\nu\,\mathrm{d}A = -\frac{1}{2}\int_{\partial S}\nabla f\cdot\nu\,\mathrm{d}A$. This is the case $j = 2$. More generally, for $j = 2k$ with $k \in \mathbb{N}_{\geq 2}$, we use that (for $x \in \partial S$), $\tilde{u}^+$ satisfies $\partial_t^2\tilde{u}^+(t,x) = \Delta\tilde{u}^+(t,x) + O(t^\infty)$. Equation 15 ensures that as $t \to 0^+$,

$$h^{(2k)}(t) = \int_{\partial S}\nabla(\Delta^{k-1}\tilde{u}^+(t,\cdot))\cdot\nu\,\mathrm{d}A + O(t^\infty).$$

As for the case $k = 1$, it follows that $h^{(2k)}(0) = -\int_{\partial S}\nabla(\Delta^{k-1}a_0^+)\cdot\nu\,\mathrm{d}A$, the divergence theorem yields the claim. □

The odd coefficients are trickier, we only compute the case $j = 3$. We start with the observation that for $x \in \partial S$, $\varphi^+(t,x) = t$ and therefore

$$\tilde{u}^+(t,x) = \sum_{i=0}^{N}\frac{1}{i!}t^i a_i^+(t,x) \quad \text{for} \;\; t \geq 0, \;\; x \in \partial S.$$

Recall that the Lie-derivative acts on functions $w \in C^\infty(M)$ by $\mathcal{L}_\nu w = \nabla w \cdot \nu$. Thus $\mathcal{L}_\nu \theta_{i+1}(\varphi^+(t,x)) = -\theta_i(\varphi^+(t,x))$, so for $x \in \partial S$,

$$\mathcal{L}_\nu \tilde{u}^+(t,x) = \sum_{i=0}^{N-1} \frac{t^i}{i!}(\mathcal{L}_\nu a_i^+(t,x) - a_{i+1}(t,x)) + O(t^\infty).$$

Therefore $\partial_t \mathcal{L}_\nu \tilde{u}^+(0,x) = \partial_t(\mathcal{L}_\nu a_0^+(0,x) - a_1^+(t,x)) + (\mathcal{L}_\nu a_1^+(0,x) - a_2^+(0,x))$, but the second term is zero as a_1^+ and a_2^+ vanish at $t = 0$ by Lemma 4. Substituting the transport equations and removing further zero terms leaves $\partial_t \mathcal{L}_\nu \tilde{u}^+(0,x) = \mathcal{L}_\nu L a_0^+(0,x) + \frac{1}{2}\Box a_0(0,x) = \frac{1}{2}\left(\mathcal{L}_\nu L f(x) - \frac{1}{2}\Delta f(x) + \frac{1}{2}L^2 f(x)\right)$. Thus (recall that $L = -\mathcal{L}_\nu + \frac{1}{2}\Delta\varphi$) directly from Eq. (15),

$$h^{(3)}(0) = -\frac{1}{2}\int_{\partial S} \mathcal{L}_\nu L f(x) - \frac{1}{2}\Delta f(x) + \frac{1}{2}L^2 f(x)\,\mathrm{d}A(x).$$

The formula

$$\Omega_{S,f}(t) = \int_0^\infty \hat{k}(s)\left(\int_S f\,\mathrm{d}V - h(s\sqrt{t})\right)\mathrm{d}s \tag{20}$$

established in the previous section, together with Lemma 3, yields the asymptotic behaviour of $\Omega_{S,f}(t)$ by taking the Taylor expansion of h using Corollary 5. This gives the remainder of the claims of theorem 2.

4 Discussion

The above-said is not specific to the heat equation. Taking $k(x) = \exp(-x^{2m})$, $m \in \mathbb{N}$, we may, for example, study the one-parameter operator family $\exp(-t^m\Delta^m)$. The wave equation estimates needed are the same. For $m \geq 2$, a brief calculation yields the explicit $t \to 0^+$ asymptotics

$$\langle \exp(t^m\Delta^m) f \mathbb{1}_S, \mathbb{1}_S\rangle = \int_S f\,\mathrm{d}V - \left(\pi^{-1}\Gamma\left(\frac{2m-1}{2m}\right)\int_{\partial S} f\,\mathrm{d}A\right)\sqrt{t} + o(t).$$

We conclude with the observation that the generalization of this paper to *weighted* Riemannian manifolds (cf. [4]) is straightforward.

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