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ON THE CORNER CONTRIBUTIONS TO THE HEAT COEFFICIENTS OF GEODESIC POLYGONS

by Dorothee SCHUETH

This paper is dedicated to the memory of Marcel Berger.

Abstract. — Let $\mathcal{O}$ be a compact Riemannian orbisurface. We compute formulas for the contribution of cone points of $\mathcal{O}$ to the coefficient at t^2 of the asymptotic expansion of the heat trace of $\mathcal{O}$, the contributions at t^0 and t^1 being known from the literature. As an application, we compute the coefficient at t^2 of the contribution of interior angles of the form $\gamma = \pi/k$ in geodesic polygons in surfaces to the asymptotic expansion of the Dirichlet heat kernel of the polygon, under a certain symmetry assumption locally near the corresponding corner. The main novelty here is the determination of the way in which the Laplacian of the Gauss curvature at the corner point enters into the coefficient at t^2. We finish with a conjecture concerning the analogous contribution of an arbitrary angle γ in a geodesic polygon.

Résumé. — Soit $\mathcal{O}$ une orbisurface riemannienne compacte. Nous calculons des formules pour la contribution des singularités coniques de $\mathcal{O}$ au coefficient de t^2 du développement asymptotique de la trace du noyau de la chaleur de $\mathcal{O}$, les contributions de t^0 et t^1 étant connues. Comme application, nous calculons le coefficient de t^2 de la contribution d'un angle intérieur de la forme $\gamma = \pi/k$ dans un polygone géodésique sur une surface au développement asymptotique du noyau de la chaleur de Dirichlet du polygone, sous une hypothèse locale de symétrie près du sommet correspondant. La principale nouveauté ici est la détermination de la façon dont le Laplacien de la courbure de Gauss au sommet en question entre dans le coefficient de t^2. Nous terminons par une conjecture concernant la contribution analogue d'un angle γ arbitraire dans un polygone géodésique.

1. Introduction

This paper concerns the influence of certain singularities on the heat coefficients. The systematic study of heat coefficients in the context of smooth

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Riemannian manifolds started in the 1960s. Let (M^d, g) be a closed and connected Riemannian manifold, $\Delta_g = -\operatorname{div}_g \circ \operatorname{grad}_g$ the associated Laplace operator, and $H : (0,\infty) \times M \times M \to \mathbb{R}$ the corresponding heat kernel. Minakshisundaram and Pleijel [15] proved that there is an asymptotic expansion

$$H(t,p,q) \sim_{t\searrow 0} (4\pi t)^{-d/2} e^{-\operatorname{dist}^2(p,q)/4t} \sum_{\ell=0}^{\infty} \boldsymbol{u}_\ell(p,q) t^\ell$$

for (p,q) in some neighborhood of the diagonal in $M \times M$, and they gave recursive formulas for the functions $\boldsymbol{u}_\ell$. Correspondingly, the heat trace

$$Z : t \mapsto \int_M H(t,p,p)\,\mathrm{dvol}_g(p) = \sum_{j=0}^{\infty} e^{-t\lambda_j},$$

where $0 = \lambda_0 < \lambda_1 \leqslant \lambda_2 \leqslant \ldots \to \infty$ is the eigenvalue spectrum of Δ_g with multiplicities, admits the asymptotic expansion

$$Z(t) \sim_{t\searrow 0} (4\pi t)^{-d/2} \sum_{\ell=0}^{\infty} a_\ell t^\ell$$

with the so-called *heat coefficients*

$$a_\ell := \int_M \boldsymbol{u}_\ell(p,p)\,\mathrm{dvol}_g(p)\,.$$

Each of the coefficients a_ℓ in this expansion is a spectral invariant in the sense that it is determined by the eigenvalue spectrum of Δ_g . Here, $\boldsymbol{u}_0 = 1$ and a_0 is just the volume of (M,g).

Formulas for a_1 and a_2 (more precisely, even for $\boldsymbol{u}_1(p,p)$ and $\boldsymbol{u}_2(p,p)$) were first given by Marcel Berger in his announcement [2] of 1966. One has

$$\boldsymbol{u}_1(p,p) = \frac{1}{6}\operatorname{scal}_g(p)\,,$$

where scal_g denotes the scalar curvature associated with g. Although Berger called that formula “folklore”, he was the first to publish a proof of it, in 1968, in his paper [3]. In the same paper, he proved the formula

$$\boldsymbol{u}_2(p,p) = \frac{1}{360}(5\operatorname{scal}_g^2 - 2\|\mathrm{ric}_g\|^2 + 2\|R_g\|^2 - 12\Delta_g \operatorname{scal}_g)(p),$$

where ric_g and R_g denote the Ricci and the Riemannian curvature tensor, respectively. This formula was considerably more intricate to derive than that for $\boldsymbol{u}_1(p,p)$. Berger’s method was a direct calculation in local coordinates, using Minakshisundaram/Pleijel’s recursive formulas for the $\boldsymbol{u}_\ell$. Meanwhile, in 1967, McKean and Singer [14] had found a shorter way of deriving the corresponding formula for a_2 . However, this did not provide an alternative proof of Berger’s full formula for $\boldsymbol{u}_2(p,p)$ (which will actually be needed in the present paper): Its last term is not visible in a_2 since the integral over $\Delta_g \operatorname{scal}_g$ vanishes.

In 1971, Sakai computed a_3 using an approach much similar to Berger's. Later, Gilkey computed formulas for heat coefficients in more general contexts like Schrödinger operators on vector bundles and, together with Branson, for manifolds with smooth boundary (see [6, 10]). For nonempty boundary, also half-powers of t can occur in the asymptotic expansion of the corresponding heat trace (with, e.g., Dirichlet or Neumann boundary conditions). On the other hand, also surfaces with corners (albeit only in the case of polygons in euclidean $\mathbb{R}^2$) were considered as early as 1966 in Kac's famous paper [12], where it was shown that the Dirichlet heat trace satisfies

$$Z(t) = (4\pi t)^{-1} \operatorname{vol}(M) - (4\pi t)^{-1/2} \cdot \frac{1}{4} \operatorname{vol}(\partial M) + \sum_{i=1}^{N} \frac{\pi^2 - \gamma_i^2}{24\gamma_i \pi} + O(t^\infty) \tag{1.1}$$

for $t \searrow 0$, where $\gamma_1, \ldots, \gamma_N$ are the interior angles of the polygon. Actually, Kac's formula for the angle contribution was more complicated; McKean and Singer brought it into the above form in their paper [14] of 1967, using an unpublished formula of D. Ray. A full proof of (1.1) was given in 1988 by van den Berg and Srisatkunarajah [1]. In 2005, Watson [19] computed the heat coefficients for geodesic polygons in the round two-sphere; in 2017, Uçar [18] achieved the same for the more difficult case of geodesic polygons in the hyperbolic plane. Here, in contrast to the flat case, the asymptotic expansion of $Z(t)$ does not break off as in (1.1), and there are infinitely many coefficients involving contributions from the corners. More precisely, for a geodesic polygon in a surface of constant curvature K, the contribution of an interior angle γ to the small-time asymptotic expansion of $Z(t)$ has the form

$$\sum_{\ell=0}^{\infty} e_\ell(\gamma) K^\ell t^\ell\,; \tag{1.2}$$

see [18, Corollary 3.37], including explicit formulas for the $e_\ell(\gamma)$. As an application, Uçar proved that for constant $K \neq 0$, the set of angles of a geodesic polygons, including multiplicities, is spectrally determined ([18, Theorem 3.40]).

While (1.2) just turned out from Watson's and Uçar's direct computations, Uçar also gave, in the special case that γ is of the form $\gamma = \pi/k$, a conceptual proof of the fact that the coefficient at t^ℓ must be of the form $e_\ell(\gamma)K^\ell$. Note that this cannot be achieved by just rescaling, since K

can be either positive or negative. For his reasoning, Uçar used a qualitative description (involving curvature invariants) by Donnelly [8] and Dryden et al. [9] concerning the contribution of orbifold singularities to the heat coefficients of Riemannian orbifolds. He showed that the heat coefficient contributions of a corner with interior angle $\gamma = \pi/k$ in a geodesic polygon of constant curvature with Dirichlet boundary conditions can be viewed, in a sense, as the difference between the contributions of an orbifold cone point of order k and a dihedral orbifold singularity with isostropy group of order $2k$; see [18, p. 142–144]. Since those two contributions are, by Donnelly's structural theory, known to be determined by $\gamma = \pi/k$ and curvature invariants of appropriate order, and since the only curvature invariant of order 2ℓ in the case of constant curvature is K^ℓ, this implies that the coefficients must be of the form $e_\ell(\gamma)K^\ell$ here.

The present paper constitutes a first step into studying corner contributions in the setting of geodesic polygons in surfaces of *nonconstant* curvature. Under a certain symmetry assumption around the corresponding corner p (see (5.1)), we show in our Main Theorem 5.3 that the contribution of an interior angle of the form $\gamma = \pi/k$ to the small-time asymptotic expansion of the Dirichlet heat trace of the polygon is of the form

$$\sum_{t=0}^{\infty} c_\ell(\gamma)t^\ell$$

with

$$c_0(\gamma) = \frac{\pi^2 - \gamma^2}{24\gamma\pi}, \quad c_1(\gamma) = \left(\frac{\pi^4 - \gamma^4}{720\gamma^2\pi} + \frac{\pi^2 - \gamma^2}{72\gamma\pi}\right) K(p),$$

and

$$(1.3) \quad c_2(\gamma) = \left(\frac{\pi^6 - \gamma^6}{5040\gamma^5\pi} + \frac{\pi^4 - \gamma^4}{1440\gamma^3\pi} + \frac{\pi^2 - \gamma^2}{360\gamma\pi}\right) K(p)^2 \\ - \left(\frac{\pi^6 - \gamma^6}{30240\gamma^5\pi} + \frac{\pi^4 - \gamma^4}{2880\gamma^3\pi} + \frac{\pi^2 - \gamma^2}{360\gamma\pi}\right) \Delta_g K(p),$$

with our sign convention $\Delta_g = -\operatorname{div}_g \circ \operatorname{grad}_g$. The coefficient $c_0(\gamma)$ is not new (see [13]); moreover, $c_1(\gamma)$ and the coefficient at $K(p)^2$ in (1.3) coincide, of course, with Uçar's corresponding formulas for constant curvature. The main novelty here is the coefficient at $\Delta_g K(p)$ in (1.3) which, of course, did not appear in the constant curvature case. We conjecture that these formulas generalize to the case of arbitrary $\gamma \in (0, 2\pi]$ under the assumption that the Hessian of K at p is a multiple of the metric (Conjecture 5.5).

Our strategy for proving the Main Theorem again uses orbifold theory. For a cone point $\overline{p}$ of order k in a closed Riemannian orbisurface $(\mathcal{O}, g)$

we compute the coefficient $a_2^{(\{\bar{p}\})}$ at t^2 of its contribution to the heat trace of $(\mathcal{O}, g)$ (Theorem 4.1), the coefficients at t^0 and t^1 being known from the literature [8], [9] (see Remark 4.2). We then show that under the symmetry assumption (5.1) from 5.1, each $c_\ell(\pi/k)$ is just $\frac{1}{2}$ times the corresponding $a_\ell^{(\{\bar{p}\})}$ (Remark 5.2); this implies our Main Theorem 5.3. In turn, to prove Theorem 4.1 we first compute the coefficient $b_2(\Phi)$ at t^2 in Donnelly's asymptotic expansion of the integral of $H(t, \cdot, \Phi(\cdot))$ over a small neighborhood of p in a surface (M, g), where Φ is an isometry of a (slightly bigger) neighborhood whose differential at p is a rotation by an angle $\varphi \in (0, \pi]$ (Theorem 3.7); we then use a formula from [9] (see (4.1)). For the computation of $b_2(\Phi)$, we closely follow Donnelly's proof of the existence of the mentioned asymptotic expansion (in a much more general setting) from [8]. In preparation for that, we have to give expansions for $r \searrow 0$ of $r \mapsto \boldsymbol{u}_0(\exp_p(ru), \Phi(\exp_p(ru)))$ (up to order the order of r^4) and of $r \mapsto \boldsymbol{u}_1(\exp_p(ru), \Phi(\exp_p(ru))$ (up to the order of r^2), where $u \in T_pM$ is a unit vector (Lemma 3.6). Moreover, we need the expansion of the Riemannian distance $\operatorname{dist}(\exp_p(ru), \Phi(\exp_p(ru)))$ up to the order of r^6 (Corollary 2.4, Lemma 3.4). Since a formula for the sixth order expansion of the distance funcion did not seem to be available in the literature, we first give a general formula for the sixth order expansion of $\operatorname{dist}^2(\exp_p(x), \exp_p(y))$ in surfaces, where x, y are tangent vectors at p (Lemma 2.3). For the proof, we partly follow an approach by Nicolaescu [16] which uses a Hamilton–Jacobi equation for $\operatorname{dist}^2(q, \cdot)$.

This paper is organized as follows: In Section 2, we provide some notation and technical preparations, among these the sixth order expansion of the distance function in surfaces (Lemma 2.3 and Corollary 2.4; the proof of Lemma 2.3 is postponed to the Appendix). In Section 3, we first prove Lemma 3.6 concerning the mentioned expansions of $\boldsymbol{u}_0$ and $\boldsymbol{u}_1$; we then deduce Theorem 3.7 concerning $b_2(\Phi)$ by following Donnelly's approach. Section 4 is devoted to the computation of $a_2^{(\{\bar{p}\})}$ for cone points of order k in orbisurfaces (Theorem 4.1), using Theorem 3.7 and Dryden et al.'s formula (4.1). In Section 5 we prove our Main Theorem 5.3; we conclude with some remarks and Conjecture 5.5.

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of the inspiration for the results in this article was provided by having a closer look, for that occasion, at Berger's seminal early works [2], [3], [4], [5] in spectral geometry, and also by his fearless use of a bit of "calcul brutal" when needed (quotation from the first line of p. 923 in [3]).

2. Preliminaries

In this paper, (M, g) will always denote a two-dimensional Riemannian manifold and $K : M \to \mathbb{R}$ its Gauss curvature. Let $\Delta_g = -\operatorname{div}_g \circ \operatorname{grad}_g$ be the Laplace operator on smooth functions on M. By $\nabla^2 K$ we denote the Hessian tensor of K; that is, $\nabla^2 K_p(x, y) = g_p(\nabla_x \operatorname{grad}_g K, y)$ for $x, y \in T_pM$, where ∇ denotes the Levi-Civita connection. In particular, if $\{u, \widetilde{u}\}$ is an orthonormal basis of T_pM then

$$\Delta_g K(p) = -\nabla^2 K_p(u, u) - \nabla^2 K_p(\widetilde{u}, \widetilde{u}).$$

Notation and Remarks 2.1. — Let $p \in M$ and $u \in T_pM$ with $\|u\| = 1$.

(i) If $\widetilde{u} \in T_pM$ is a unit vector with $\widetilde{u} \perp u$ and J the Jacobi field along the geodesic γ_u with $J(0) = 0$, $J'(0) = \widetilde{u}$, then

$$\ell_u(r) := \|(d\exp_p)_{ru}(r\widetilde{u})\| = \|J(r)\|$$

has the following well-known expansion for $r \searrow 0$:

$$\begin{aligned}\ell_u(r) = r - \frac{1}{6}K(p)r^3 - \frac{1}{12}\mathrm{d}K_p(u)r^4 \\ + \left(\frac{1}{120}K(p)^2 - \frac{1}{40}\nabla^2 K_p(u, u)\right) r^5 + O(r^6).\end{aligned} \tag{2.1}$$

This follows from the Jacobi equation $J'' = -(K \circ \gamma_u)J$ for Jacobi fields orthogonal to $\dot{\gamma}_u$.

(ii) For small $r > 0$, we denote by $\theta_u(r)$ the so-called volume density or area distortion of $\exp_p$ at $ru \in T_pM$. In other words, $\theta_u(r) = (\det g_{ij}(ru))^{1/2}$ in normal coordinates around p. Since $\exp_p$ is a radial isometry and we are in dimension two, we have

$$\theta_u(r) = \ell_u(r)/r.$$

Thus (2.1) implies:

$$\begin{aligned}\theta_u(r) = 1 - \frac{1}{6}K(p)r^2 - \frac{1}{12}\mathrm{d}K_p(u)r^3 \\ + \left(\frac{1}{120}K(p)^2 - \frac{1}{40}\nabla^2 K_p(u, u)\right) r^4 + O(r^5).\end{aligned} \tag{2.2}$$

(iii) For $\ell \in \mathbb{N}_0$, let $\boldsymbol{u}_\ell$ denote the (universal) functions, defined on some neighborhood of the diagonal in $M \times M$, which in case of closed surfaces appear in the asymptotic expansion of the heat kernel of (M, g):

$$H(t,p,q) \sim (4\pi t)^{-1} \exp(-\operatorname{dist}^2(p,q)/4t) \cdot \sum_{\ell=0}^{\infty} \boldsymbol{u}_\ell(p,q) t^\ell \quad \text{as} \quad t \searrow 0,$$

where $\operatorname{dist} : M \times M \to \mathbb{R}$ denotes Riemannian the distance function of (M, g).

(iv) It is well-known that $\boldsymbol{u}_0 = \theta^{-1/2}$ (see [15]); more precisely,

$$\boldsymbol{u}_0(p, \exp_p(ru)) = \theta_u(r)^{-1/2}$$

for small $r \geqslant 0$. In particular, (2.2) implies

$$\begin{aligned} \boldsymbol{u}_0(p, \exp_p(ru)) = 1 + \frac{1}{12} K(p) r^2 + \frac{1}{24} \mathrm{d}K_p(u) r^3 \\ + \left(\frac{1}{160} K(p)^2 + \frac{1}{80} \nabla^2 K_p(u,u) \right) r^4 + O(r^5). \end{aligned} \tag{2.3}$$

(v) As proved in [3] by Marcel Berger, the restriction of $\boldsymbol{u}_2$ to the diagonal is given by

$$\boldsymbol{u}_2(p,p) = \frac{1}{72} \operatorname{scal}^2(p) - \frac{1}{180} \|\mathrm{ric}_p\|^2 + \frac{1}{180} \|R_p\|^2 - \frac{1}{30} \Delta_g \operatorname{scal}(p),$$

where scal, ric, R denote the scalar curvature, the Ricci and the Riemannian curvature tensor, respectively. Recall our choice of sign for $\Delta_g = -\operatorname{div}_g \circ \operatorname{grad}_g$. In dimension two, the above formula simplifies to

$$\boldsymbol{u}_2(p,p) = \frac{1}{15} K(p)^2 - \frac{1}{15} \Delta_g K(p). \tag{2.4}$$

Lemma 2.2. — *In the notation of 2.1,*

$$\begin{aligned} \boldsymbol{u}_1(p, \exp_p(ru)) = \frac{1}{3} K(p) + \frac{1}{6} \mathrm{d}K_p(u) r \\ + \left(\frac{1}{30} K(p)^2 - \frac{1}{120} \Delta_g K(p) + \frac{1}{20} \nabla^2 K_p(u,u) \right) r^2 + O(r^3) \end{aligned} \tag{2.5}$$

for $r \searrow 0$.

Proof. — One way to obtain this is specializing Sakai's formulas (3.7), (4.3)–(4.5) from [17] (for arbitrary dimension n) to dimension two and then translating into our notation. An alternative proof which uses the two-dimensional setting right away is as follows: By Minakshisundaram/Pleijel's recursion formula from [15] for the $\boldsymbol{u}_\ell$, applied to $\ell = 1$,

$$\begin{aligned}(2.6)\quad &\boldsymbol{u}_1(p, \exp_p(ru))\\ &= -\boldsymbol{u}_0(p, \exp(ru)) \int_0^1 \boldsymbol{u}_0(p, \exp_p(tru))^{-1} \left(\Delta_g \boldsymbol{u}_0(p, \,\cdot\,)\right)(\exp_p(tru))\,\mathrm{d}t.\end{aligned}$$

For small $r > 0$, the curvature of the distance sphere $\partial B_r(p)$ at $\exp_p(ru)$ is

$$\frac{1}{r} + \frac{\theta_u'(r)}{\theta_u(r)} = \frac{1}{r} - \frac{1}{3}K(p)r + O(r^2),$$

where the latter equation holds by (2.2). Moreover, letting $\widetilde{u}$ be a unit vector orthogonal to u and

$$u(s) := \cos(s)u + \sin(s)\widetilde{u},$$

the curve $c : t \mapsto \exp_p(ru(t/\ell_u(r)))$ satisfies $c(0) = \exp_p(ru)$, $\|\dot{c}(0)\| = 1$ and

$$\left\langle \frac{D}{\mathrm{d}t}\dot{c}(0), \dot{c}(0) \right\rangle = \frac{1}{2} \cdot \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \ell_{u(t/\ell_u(r))}(r)^2/\ell_u(r)^2.$$

Using (2.1), one can check that the latter expression is of order $O(r^2)$ for $r \searrow 0$. Thus, for any function f near p which is of the form

$$f(\exp_p(ru)) = \alpha(r)\beta(u)$$

with smooth $\alpha : [0, \varepsilon) \to \mathbb{R}$ and $\beta : S_p^1 \to \mathbb{R}$, where $S_p^1 \subset (T_pM, g_p)$ denotes the unit circle, one has

$$\begin{aligned}(2.7)\quad (\Delta_g f)(\exp_p(ru)) = &-\left[\alpha''(r) + \left(\frac{1}{r} - \frac{1}{3}K(p)r + O(r^2)\right)\alpha'(r)\right]\beta(u)\\ &- \alpha(r)\left(\frac{1}{\ell_u(r)^2}\nabla^2\beta_u(\widetilde{u}, \widetilde{u}) + \frac{O(r^2)}{\ell_u(r)}d\beta_u(\widetilde{u})\right),\end{aligned}$$

where $\nabla^2\beta$ here denotes the Hessian of β as a function on the circle S_p^1. Viewing $u \mapsto \mathrm{d}K_p(u)$, $u \mapsto \nabla^2 K_p(u, u)$ in formula (2.3) as functions on S_p^1 (not on T_pM), we can apply (2.7) to the three nonconstant terms in (2.3). Evaluating up to the order of r^2 gives

$$\left(\Delta_g \boldsymbol{u}_0(p, \,\cdot\,)\right)(\exp_p(ru)) = A_1 + A_2 + A_3 + O(r^3),$$

where

$$
\begin{aligned}
A_1 &= -\frac{1}{12}K(p)\left(2+2-\frac{2}{3}K(p)r^2\right) = -\frac{1}{3}K(p) + \frac{1}{18}K(p)^2r^2,\\
A_2 &= -\frac{1}{24}\left(\mathrm{d}K_p(u)(6r+3r) - r\cdot \mathrm{d}K_p(u)\right) = -\frac{1}{3}\mathrm{d}K_p(u)r\\
A_3 &= -\left(\frac{1}{160}K(p)^2 + \frac{1}{80}\nabla^2 K_p(u,u)\right)(12r^2+4r^2)\\
&\qquad -\frac{1}{80}r^2\left(2\nabla^2K_p(\widetilde{u},\widetilde{u}) - 2\nabla^2K_p(u,u)\right)\\
&= -\left(\frac{1}{10}K(p)^2 + \frac{7}{40}\nabla^2K_p(u,u) + \frac{1}{40}\nabla^2K_p(\widetilde{u},\widetilde{u})\right)r^2\\
&= \left(-\frac{1}{10}K(p)^2 + \frac{1}{40}\Delta_g K(p) - \frac{3}{20}\nabla^2K_p(u,u)\right)r^2.
\end{aligned}
$$

Thus,

$$
\begin{aligned}
\left(\Delta_g \boldsymbol{u}_0(p,\,\cdot\,)\right)\left(\exp_p(ru)\right) &= -\frac{1}{3}K(p) - \frac{1}{3}\mathrm{d}K_p(u)r\\
&\quad + \left(-\frac{2}{45}K(p)^2 + \frac{1}{40}\Delta_g K(p) - \frac{3}{20}\nabla^2K_p(u,u)\right)r^2 + O(r^3).
\end{aligned}
$$

By this and (2.3),

$$
\begin{aligned}
\left(\Delta_g \boldsymbol{u}_0(p,\,\cdot\,)/\boldsymbol{u}_0(p,\,\cdot\,)\right)\left(\exp_p(ru)\right) &= -\frac{1}{3}K(p) - \frac{1}{3}\mathrm{d}K_p(u)r\\
&\quad + \left(-\frac{1}{60}K(p)^2 + \frac{1}{40}\Delta_g K(p) - \frac{3}{20}\nabla^2K_p(u,u)\right)r^2 + O(r^3).
\end{aligned}
$$

The integral in (2.6) thus gives

$$
-\frac{1}{3}K(p) - \frac{1}{6}\mathrm{d}K_p(u)r + \left(-\frac{1}{180}K(p)^2 + \frac{1}{120}\Delta_g K(p) - \frac{1}{20}\nabla^2K_p(u,u)\right)r^2 + O(r^3).
$$

Multiplying this by $-\boldsymbol{u}_0(p,\exp_p(ru)) = -1 - \frac{1}{12}K(p)r^2 + O(r^3)$ (see (2.3)), we obtain the desired formula. $\square$

Lemma 2.3. — *As above, let* dist : $M \times M \to \mathbb{R}$ *be the Riemannian distance function on the surface* (M,g)*. Then for all* $x, y \in T_pM$*,*

$$\begin{aligned}(2.8)\quad \mathrm{dist}^2(\exp_p(x),\exp_p(y)) &= \|x-y\|^2 - \frac{1}{3}K(p)\|x\wedge y\|^2 \\ &- \frac{1}{12}\mathrm{d}K_p(x+y)\|x\wedge y\|^2 - \frac{1}{45}K(p)^2\left(\|x\|^2 - 4\langle x,y\rangle + \|y\|^2\right)\|x\wedge y\|^2 \\ &- \frac{1}{60}\left(\nabla^2K_p(x,x)+\nabla^2K_p(x,y)+\nabla^2K_p(y,y)\right)\|x\wedge y\|^2 + o((\|x\|^2+\|y\|^2)^3).\end{aligned}$$

We postpone the proof of Lemma 2.3 to the Appendix.

Corollary 2.4. — *Let* $u \neq v$ *be vectors in the unit sphere* $S^1_p \subset T_pM$*. Let* $\varphi := \arccos\langle u,v\rangle \in (0,\pi]$ *denote the angle between* u *and* v*. Then, using the abbreviation* $C := \|u-v\| = \sqrt{2-2\cos\varphi}$*, we have*

$$\begin{aligned}\mathrm{dist}(\exp_p(ru),\exp_p(rv)) &= Cr - \frac{\sin^2\varphi}{6C}K(p)r^3 - \frac{\sin^2\varphi}{24C}\mathrm{d}K_p(u+v)r^4 \\ &- \left[\left(\frac{\sin^4\varphi}{72C^3} + \frac{\sin^2\varphi\cdot(2-4\cos\varphi)}{90C}\right)K(p)^2\right. \\ &\left.+\frac{\sin^2\varphi}{120C}\left(\nabla^2K_p(u,u)+\nabla^2K_p(u,v)+\nabla^2K_p(v,v)\right)\right]r^5 \\ &- \frac{\sin^4\varphi}{144C^3}K(p)\mathrm{d}K_p(u+v)r^6 + O(r^7)\end{aligned}$$

for $r \searrow 0$.

Proof. — Note that $\|ru \wedge rv\|^2 = r^4\sin^2\varphi$. The claimed formula now follows directly by applying Lemma 2.3 to $x := ru$, $y := rv$ and forming the square root of the resulting power series. □

3. Donnelly's b_2 for rotations in dimension two

Notation and Remarks 3.1. — We continue to use the notation of Section 2; in particular, (M,g) is a two-dimensional Riemannian manifold. Let $p \in M$ and $\varphi \in (0,\pi]$. Equip T_pM with an arbitrarily chosen orientation, and let $D^\varphi : T_pM \to T_pM$ denote the corresponding euclidean rotation by the angle φ. Let $\varepsilon_1 > 0$ such that $\exp_p$ is a diffeomorphism from $B_{\varepsilon_1}(0_p) \subset T_pM$ to its image $B := B_{\varepsilon_1}(p) \subset M$. Choose $0 < \varepsilon < \varepsilon_2 < \varepsilon_1$, and let

$$V := B_{\varepsilon_2}(p) \subset B \quad\text{and}\quad U := B_\varepsilon(p) \subset V.$$

Suppose that there exists an isometry

$$\Phi : (B, g) \to (B, g) \quad \text{with } \Phi(p) = p \text{ and } d\Phi_p = D^{\varphi}.$$

A result by Donnelly [8], applied to this special situation, says that

$$I(t) := \int_U H(t, q, \Phi(q)) \, \mathrm{dvol}_g(q)$$

admits an asymptotic expansion of the form

$$I(t) \sim \sum_{\ell=0}^{\infty} b_\ell(\Phi) t^\ell \text{ for } t \searrow 0, \tag{3.1}$$

where $H := H_V$ denotes the (Dirichlet) heat kernel of V.

Remark 3.2. — Note that no factor $(4\pi t)^{-n/2}$ is visible on the right hand side of (3.1); this is due to the fact that the dimension n of the fixed point set $\{p\}$ of Φ is zero here. In a much more general situation, involving fixed point sets of arbitrary isometries on manifolds of arbitrary dimension, Donnelly proved a structural result for analogous coefficients b_ℓ and explicitly computed b_0 and b_1 (but not b_2). In our above situation, Donnelly's formulas for b_0 and b_1 amount to

$$b_0(\Phi) = (2 - 2\cos\varphi)^{-1} \text{ and } b_1(\Phi) = 2K(p)(2 - 2\cos\varphi)^{-2}$$

(see also [9] for this in the case $\varphi \in \{2\pi/k \mid k \in \mathbb{N}\}$). In this section we will compute $b_2(\Phi)$; see Theorem 3.7. Our strategy is to follow Donnelly's general approach from [8, p. 166–167], in our special setting.

Remark 3.3.

(i) The coefficients in (3.1) will not change if in the definition of $I(t)$ we replace V by any other open, relatively compact, smoothly bounded neighborhood of $\overline{U}$ in M (e.g., M itself in case M is a closed surface). In fact, while the individual values of $H(t, q, w)$ will of course depend on this choice (and so will $I(t)$), the coefficients of the small-time expansion of $H(t, q, w)$ for $q, w \in U$ do not depend on it. This is due to the "Principle of not feeling the boundary"; see, e.g., [11], [12], or [18, Lemma 3.17].

(ii) The coefficients in (3.1) will not change, either, if in the definition of $I(t)$ we replace the integral over U by the integral over any smaller open neighborhood $\widetilde{U} \subset U$ of p. This is due to the fact that by our choices of ε and φ, the function $U \setminus \widetilde{U} : q \mapsto \mathrm{dist}(q, \Phi(q)) \in \mathbb{R}$ will be bounded below by some positive constant, which implies that the integral of $H(t, q, \Phi(q))$ over $U \setminus \widetilde{U}$ vanishes to infinite order as $t \searrow 0$.

Lemma 3.4. — *Let the situation be as in 3.1. Then we have* $\mathrm{d}K_p = 0$. *Moreover, if* $\varphi \in (0,\pi)$ *then* $\nabla^2 K_p = -\frac{1}{2}\Delta_g K(p)\cdot g_p$. *Finally, for every* $\varphi \in (0,\pi]$ *and every* $u \in S^1_p$, *the function*

$$d_u : r \mapsto \operatorname{dist}(\exp_p(ru), \exp_p(rv)),$$

where $v := D^\varphi(u)$, *satisfies*

$$\begin{aligned}(3.2)\quad d_u(r) = Cr - \frac{\sin^2\varphi}{6C}K(p)r^3 \\ - \left[\left(\frac{\sin^4\varphi}{72C^3} + \frac{\sin^2\varphi\cdot(2-4\cos\varphi)}{90C}\right)K(p)^2 - \frac{\sin^2\varphi\cdot(2+\cos\varphi)}{240C}\Delta_g K(p)\right]r^5 \\ + O(r^7)\end{aligned}$$

for $r \searrow 0$, *where* $C = \sqrt{2-2\cos\varphi}$.

Proof. — The first two statements are clear since $\mathrm{d}K_p$ and $\nabla^2 K_p$ are invariant under D^φ. In particular, in the case $\varphi \in (0,\pi)$ we have

$$\nabla^2 K_p(u,u) + \nabla^2 K_p(u,v) + \nabla^2 K_p(v,v) = -\frac{1}{2}\Delta_g K(p)\cdot(2+\cos\varphi),$$

so (3.2) follows by Corollary 2.4. In case $\varphi = \pi$, (3.2) trivially holds by $d_u(r) = 2r$, $C = 2$, $\sin\varphi = 0$. □

Remark 3.5. — In the following Lemma 3.6 some formulas would become simpler if we assumed $\nabla^2 K_p$ to be a multiple of g_p. This would imply $\nabla^2 K_p(u,u) = -\frac{1}{2}\Delta_g K(p)$ for all $u \in S^1_p$. Recall from Lemma 3.4 that this is the case anyway if $\varphi \in (0,\pi)$ in 3.1. For $\varphi = \pi$, however, the above assumption on $\nabla^2 K_p$ would unnecessarily make the Lemma less precise.

Lemma 3.6. — *In the situation of 3.1, letting* $C := \sqrt{2-2\cos\varphi}$ *and* $v := D^\varphi u$ *we have*

$$\begin{aligned}\boldsymbol{u}_0(\exp_p(ru), \exp_p(rv)) = 1 + \frac{1}{12}K(p)d_u(r)^2 \\ + \left(\frac{1}{24C^2}\nabla^2 K_p(u,u) + \frac{1}{160}K(p)^2 - \frac{1}{120}\nabla^2 K_p(u,u)\right)d_u(r)^4 \\ + O(d_u(r)^5),\end{aligned}$$

$$\begin{aligned}\boldsymbol{u}_1(\exp_p(ru), \exp_p(rv)) = \frac{1}{3}K(p) \\ + \left(\frac{1}{6C^2}\nabla^2 K_p(u,u) + \frac{1}{30}K(p)^2 - \frac{1}{30}\nabla^2 K_p(u,u) - \frac{1}{120}\Delta_g K(p)\right)d_u(r)^2 \\ + O(d_u(r)^3),\end{aligned}$$

$$\boldsymbol{u}_2(\exp_p(ru), \exp_p(rv)) = \frac{1}{15}K(p)^2 - \frac{1}{15}\Delta_g K(p) + O(d_u(r)^1).$$

Proof. — Let $q(r) := \exp_p(ru)$, $w(r) := \exp(rv)$. Moreover, for small $r \geqslant 0$, let $Y(r) \in T_{q(r)}M$ be the vector with $\exp_{q(r)}(Y(r)) = w(r)$. Then $\|Y(r)\|_g = d_u(r)$, $Y(0) = 0$, and the initial covariant derivative of Y is

$$Y'(0) = D^\varphi u - u = (\cos\varphi - 1)u + (\sin\varphi)\widetilde{u} = -\frac{1}{2}C^2 u + (\sin\varphi)\widetilde{u},$$

where $\widetilde{u} := D^{\pi/2}u$. We apply (2.3) to $q(r)$ instead of p and $d_u(r)$ instead of r, and we use $\mathrm{d}K_p = 0$ (see Lemma 3.4). Recalling (3.2) and, in particular, $r = O(d_u(r))$ for $r \searrow 0$ (since $C > 0$), we obtain

$$\begin{aligned}
\boldsymbol{u}_0(q(r), w(r)) &= 1 + \frac{1}{12}K(q(r))d_u(r)^2 + \frac{1}{24}\mathrm{d}K_{q(r)}(Y(r))d_u(r)^2 \\
&\quad + \frac{1}{160}K(q(r))^2 d_u(r)^4 + \frac{1}{80}\nabla^2 K_{q(r)}(Y(r), Y(r))d_u(r)^2 + O(d_u(r)^5) \\
&= 1 + \frac{1}{12}(K(p) + \frac{1}{2}r^2\nabla^2 K_p(u,u))d_u(r)^2 + \frac{1}{24}r\nabla^2 K_p(u, rY'(0))d_u(r)^2 \\
&\quad + \frac{1}{160}K(p)^2 d_u(r)^4 + \frac{1}{80}\nabla^2 K_p(rY'(0), rY'(0))d_u(r)^2 + O(d_u(r)^5).
\end{aligned}$$

We have

$$\begin{aligned}
r\nabla^2 K_p(u, rY'(0)) &= -\frac{1}{2}\nabla^2 K_p(u,u)C^2 r^2, \\
\nabla^2 K_p(rY'(0), rY'(0)) &= \nabla^2 K_p(u,u)C^2 r^2.
\end{aligned} \tag{3.3}$$

In case $\pi = \varphi$ this follows from $Y'(0) = -\frac{1}{2}C^2 u + 0$ and $C = 2$; in case $\varphi \in (0, \pi)$ it follows from the fact that $\nabla^2 K_p$ is a multiple of g_p (see Lemma 3.4) and from $\|Y'(0)\|_g^2 = C^2$. The first statement of the lemma now follows by noting that $C^2 r^2 = d_u(r)^2 + O(d_u(r)^4)$. Analogously, (2.5) and evaluating up the order of r^2 gives, using (3.3) again:

$$\begin{aligned}
\boldsymbol{u}_1(q(r), w(r)) &= \frac{1}{3}K(q(r)) + \frac{1}{6}\mathrm{d}K_{q(r)}(Y(r)) \\
&\quad + \left(\frac{1}{30}K(q(r))^2 - \frac{1}{120}\Delta_g K(q(r))\right)d_u(r)^2 + \frac{1}{20}\nabla^2 K_{q(r)}(Y(r), Y(r)) \\
&\qquad + O(d_u(r)^3) \\
&= \frac{1}{3}\left(K(p) + \frac{1}{2}r^2\nabla^2 K_p(u,u)\right) + \frac{1}{6}\cdot\left(-\frac{1}{2}\nabla^2 K_p(u,u)C^2 r^2\right) \\
&\quad + \left(\frac{1}{30}K(p)^2 - \frac{1}{120}\Delta_g K(p)\right)d_u(r)^2 + \frac{1}{20}\nabla^2 K_p(u,u)C^2 r^2 + O(d_u(r)^3),
\end{aligned}$$

which implies the second formula. The third formula is clear by (2.4). $\square$

THEOREM 3.7. — *In the situation of 3.1, and with* $C := \sqrt{2 - 2\cos\varphi}$, *the coefficient* $b_2(\Phi)$ *in* (3.1) *is given by*

$$b_2(\Phi) = \left(\frac{12}{C^6} - \frac{2}{C^4}\right) K(p)^2 - \frac{2}{C^6}\Delta_g K(p).$$

Proof. — Recall the notation of 3.1. There is a neighborhood $\Omega \subset V \times V$ of the diagonal such that for all $(q, w) \in \Omega$,

$$4\pi t\, e^{\operatorname{dist}^2(q,w)/4t} H(t, q, w) - \sum_{k=0}^{2} \boldsymbol{u}_k(q, w) t^k \in O(t^3) \text{ as } t \searrow 0,$$

and this holds locally uniformly on Ω. By Remark 3.3 (ii), we can assume that ε is so small that $(q, \Phi(q)) \in \Omega$ for all q in the closure $\overline{U} \subset V$ of $U = B_\varepsilon(p)$. Using polar coordinates on U and writing

$$\overline{H}(t, x, y) := H(t, \exp_p(x), \exp_p(y))$$

for $x, y \in B_{\varepsilon_2}(0_p)$, we have

$$I(t) = \int_{S_p^1} \int_0^\varepsilon \overline{H}(t, ru, rD^\varphi(u)) \cdot \ell_u(r)\, \mathrm{d}r\, \mathrm{d}u,$$

where ℓ_u is as in 2.1. Note that by our choices of ε and φ, the function

$$S_p^1 \times [0, \varepsilon) \ni (u, r) \mapsto d_u(r) := \operatorname{dist}(\exp_p(u), \exp_p(rD^\varphi(u))) \in \mathbb{R}$$

is continuous, and it is smooth on $S_p^1 \times (0, \varepsilon)$. By Lemma 3.4, for every $u \in S_p^1$ the function d_u has the expansion (3.2) as $r \searrow 0$. Moreover, the corresponding remainder terms for d_u, and also for d'_u, can be estimated in terms of smooth curvature expressions and are thus bounded uniformly in $u \in S_p^1$. In particular, there exists $0 < \widetilde{\varepsilon} < \varepsilon$ such that $d_u|_{[0,\widetilde{\varepsilon}]}$ has strictly positive derivative for each $u \in S_p^1$. Thus

$$\eta := \min\{d_u(\widetilde{\varepsilon}/2) \mid u \in S_p^1\} > 0$$

is a regular value of $B_{\widetilde{\varepsilon}}(p) \ni q \mapsto \operatorname{dist}(q, \Phi(q)) \in \mathbb{R}$, so

$$\rho(u) := (d_u|_{[0,\widetilde{\varepsilon}]})^{-1}(\eta) \in (0, \widetilde{\varepsilon}/2]$$

depends smoothly on $u \in S_p^1$. Let

$$\widetilde{U} := \{\exp_p(ru) \mid u \in S_p^1, r \in [0, \rho(u))\}.$$

Then $\widetilde{U} \subset U$ is an open neighborhood of p, so by Remark 3.3 (ii), $I(t)$ has the same asymptotic expansion for $t \searrow 0$ as

$$\widetilde{I}(t) := \int_{\widetilde{U}} H(t, q, \Phi(q)) = \int_{S_p^1} \int_0^{\rho(u)} \overline{H}(t, ru, rD^\varphi(u)) \cdot \ell_u(r)\, \mathrm{d}r\, \mathrm{d}u.$$

Writing d_u^{-1} for the inverse of $d_u|_{[0,\eta]}$ and substituting r by $= d_u(r)/\sqrt{t}$ we obtain

$$\tag{3.4} \widetilde{I}(t) = \int_{S_p^1}\int_0^{\eta/\sqrt{t}} \overline{H}\left(t, d_u^{-1}(z\sqrt{t})u, d_u^{-1}(z\sqrt{t})D^{\varphi}(u)\right)\cdot \\ \cdot\sqrt{t}\cdot\ell_u\left(d_u^{-1}(z\sqrt{t})\right)\cdot(d_u^{-1})'(z\sqrt{t})\,\mathrm{d}z\,\mathrm{d}u.$$

Note that

$$\operatorname{dist}\left(d_u^{-1}(z\sqrt{t})u, d_u^{-1}(z\sqrt{t})D^{\varphi}(u)\right) = z\sqrt{t}.$$

Thus, $\overline{H}\left(t, d_u^{-1}(z\sqrt{t})u, d_u^{-1}(z\sqrt{t})D^{\varphi}(u)\right)$ for $t \searrow 0$ is approximated, uniformly in $(u,z)\in S_p^1\times[0,\eta]$, by

$$\tag{3.5} (4\pi t)^{-1}e^{-z^2/4}\left(\sum_{i=0}^{2}\boldsymbol{u}_i(d_u^{-1}(z\sqrt{t})u, d_u^{-1}(z\sqrt{t})D^{\varphi}(u))t^i + O(t^3)\right).$$

By Lemma 3.6,

$$\sum_{i=0}^{2}\boldsymbol{u}_i\left(d_u^{-1}(z\sqrt{t})u, d_u^{-1}(z\sqrt{t})D^{\varphi}(u)\right)t^i = 1+\frac{1}{12}K(p)z^2t \\ +\left(\frac{1}{24C^2}\nabla^2K_p(u,u)+\frac{1}{160}K(p)^2-\frac{1}{120}\nabla^2K_p(u,u)\right)z^4t^2+\frac{1}{3}K(p)t \\ +\left(\frac{1}{6C^2}\nabla^2K_p(u,u)+\frac{1}{30}K(p)^2-\frac{1}{30}\nabla^2K_p(u,u)-\frac{1}{120}\Delta_gK(p)\right)z^2t^2 \\ +\frac{1}{15}K(p)^2t^2-\frac{1}{15}\Delta_gK(p)t^2+O(t^3),$$

uniformly in $(u,z)\in S_p^1\times[0,\eta]$. Moreover, from (3.2) one obtains

$$d_u^{-1}(s) = \frac{1}{C}s+\frac{\sin^2\varphi}{6C^5}K(p)s^3+Bs^5+O(s^7)$$

with

$$B := \left(\frac{7\sin^4\varphi}{72C^9}+\frac{\sin^2\varphi\cdot(2-4\cos\varphi)}{90C^7}\right)K(p)^2 \\ -\frac{\sin^2\varphi\cdot(2+\cos\varphi)}{240C^7}\Delta_gK(p),$$

and

$$(d_u^{-1}(s))^3 = \frac{1}{C^3}s^3 + \frac{\sin^2\varphi}{2C^7}K(p)s^5 + O(s^7),$$
$$(d_u^{-1}(s))^5 = \frac{1}{C^5}s^5 + O(s^7),$$
$$(d_u^{-1})'(s) = \frac{1}{C} + \frac{\sin^2\varphi}{2C^5}s^2 + 5Bs^4 + O(s^6).$$

Using this and (2.1), one sees by a straightforward calculation:

$$\begin{aligned}\sqrt{t}\cdot\ell_u(d_u^{-1}(z\sqrt{t}))\cdot(d_u^{-1})'(z\sqrt{t}) &= \frac{1}{C^2}zt + \left(\frac{2\sin^2\varphi}{3C^6} - \frac{1}{6C^4}\right)K(p)z^3t^2\\ &+ \left(\frac{2\sin^4\varphi}{3C^{10}} - \frac{\sin^2\varphi}{6C^8} + \frac{\sin^2\varphi\cdot(2-4\cos\varphi)}{15C^8} + \frac{1}{120C^6}\right)K(p)^2z^5t^3\\ &+ \left(-\frac{\sin^2\varphi\cdot(2+\cos\varphi)}{40C^8}\Delta_gK(p) - \frac{1}{40C^6}\nabla^2K_p(u,u)\right)z^5t^3 + O(t^4).\end{aligned}$$

By $2-4\cos\varphi = 2C^2-2$, $2+\cos\varphi = 3-\frac{1}{2}C^2$, and $\sin^2\varphi = C^2(1-\frac{1}{4}C^2)$, this becomes

$$\begin{aligned}&\sqrt{t}\cdot\ell_u(d_u^{-1}(z\sqrt{t}))\cdot(d_u^{-1})'(z\sqrt{t})\\ &= \frac{1}{C^2}zt + \left(\frac{1}{2C^4} - \frac{1}{6C^2}\right)K(p)z^3t^2 + \left(\frac{3}{8C^6} - \frac{1}{8C^4} + \frac{1}{120C^2}\right)K(p)^2z^5t^3\\ &\quad + \left[\left(-\frac{3}{40C^6} + \frac{1}{32C^4} - \frac{1}{320C^2}\right)\Delta_gK(p) - \frac{1}{40C^6}\nabla^2K_p(u,u)\right]z^5t^3 + O(t^4).\end{aligned}$$

Multiplying this expression by (3.5), we obtain that the integrand in (3.4) for $t\searrow 0$ is approximated, uniformly in $(u,z)\in S_p^1\times[0,\eta]$, by

$$\begin{aligned}\frac{1}{4\pi}e^{-z^2/4}\cdot\Bigg\{&\frac{1}{C^2}z + \left[\left(\frac{1}{2C^4} - \frac{1}{12C^2}\right)z^3 + \frac{1}{3C^2}z\right]K(p)t\\ &+ \left[\left(\frac{3}{8C^6} - \frac{1}{12C^4} + \frac{1}{1440C^2}\right)z^5 + \left(\frac{1}{6C^4} - \frac{1}{45C^2}\right)z^3 + \frac{1}{15C^2}z\right]K(p)^2t^2\\ &+ \left[\left(-\frac{3}{40C^6} + \frac{1}{32C^4} - \frac{1}{320C^2}\right)z^5 - \frac{1}{120C^2}z^3 - \frac{1}{15C^2}z\right]\Delta_gK(p)t^2\\ &+ \left[\left(-\frac{1}{40C^6} + \frac{1}{24C^4} - \frac{1}{120C^2}\right)z^5 + \left(\frac{1}{6C^4} - \frac{1}{30C^2}\right)z^3\right]\nabla^2K_p(u,u)t^2\\ &+ O(t^3)\Bigg\}.\end{aligned}$$

Recall that $\eta>0$, so for any $k\in\mathbb{N}_0$ we have $\int_{\eta/\sqrt{t}}^\infty e^{-z^2/4}z^k \in O(t^\infty)$ for $t\searrow 0$. Therefore, we can replace $\int_0^{\eta/\sqrt{t}}$ by $\int_0^\infty$ in (3.4) without changing the coefficients in its asymptotic expansion for $t \searrow 0$. Moreover,

$$\int_0^\infty e^{-z^2/4} z^{2k+1} \mathrm{d}z = 2^{2k+1} k!,$$

giving 2 for $k = 0$, 8 for $k = 1$, and 64 for $k = 2$. Finally,

$$\int_{S_p^1} \nabla^2 K_p(u,u)\,\mathrm{d}u = -\frac{1}{2}\int_{S_p^1} \Delta_g K(p)\,\mathrm{d}u.$$

Using all this, we obtain

$$\begin{aligned}
\widetilde{I}(t) = \frac{2\pi}{4\pi}\Bigg\{&\frac{1}{C^2}\cdot 2 + \left[\left(\frac{1}{2C^4} - \frac{1}{12C^2}\right)\cdot 8 + \frac{1}{3C^2}\cdot 2\right] K(p)t \\
&+ \left[\left(\frac{3}{8C^6} - \frac{1}{12C^4} + \frac{1}{1440C^2}\right)\cdot 64 + \left(\frac{1}{6C^4} - \frac{1}{45C^2}\right)\cdot 8 + \frac{1}{15C^2}\cdot 2\right] K(p)^2 t^2 \\
&+ \left[\left(-\frac{3}{40C^6} + \frac{1}{32C^4} - \frac{1}{320C^2}\right)\cdot 64 - \frac{1}{120C^2}\cdot 8 - \frac{1}{15C^2}\cdot 2\right]\Delta_g K(p) t^2 \\
&+ \left[\left(-\frac{1}{40C^6} + \frac{1}{24C^4} - \frac{1}{120C^2}\right)\cdot 64 + \left(\frac{1}{6C^4} - \frac{1}{30C^2}\right)\cdot 8\right]\cdot\left(-\frac{1}{2}\Delta_g K(p)\right)t^2\Bigg\} \\
&+ O(t^3) \\
= \frac{1}{C^2} + \frac{2}{C^4}&K(p)t + \left[\left(\frac{12}{C^6} - \frac{2}{C^4}\right)K(p)^2 - \frac{2}{C^6}\Delta_g K(p)\right]t^2 + O(t^3)
\end{aligned}$$

for $t \searrow 0$, yielding the claimed result for the coefficient $b_2(\Phi)$ at t^2 and, as an aside, the previously known formulas for $b_0(\Phi)$ and $b_1(\Phi)$ (see Remark 3.2). □

4. Contribution of orbisurface cone points to the second order heat coefficient

We now consider the heat kernel of compact Riemannian orbifolds; see, e.g., [9] for the general framework in this context. Let $(\mathcal{O}, g)$ be a closed two-dimensional Riemannian orbifold, let $H_{\mathcal{O}} : (0,\infty)\times\mathcal{O}\times\mathcal{O} \to \mathbb{R}$ denote the heat kernel associated with the Laplace operator Δ_g on $C^\infty(\mathcal{O})$, and let

$$Z(t) := \int_{\mathcal{O}} H_{\mathcal{O}}(t,x,x)\,\mathrm{d}x$$

be the corresponding heat trace. It is well-known that there is an asymptotic expansion

$$Z(t) \sim (4\pi t)^{-1}\sum_{i=0}^{\infty} a_{i/2} t^{i/2}$$

for $t \searrow 0$; half powers may occur if $\mathcal{O}$ contains mirror lines. More precisely, the principal (open) stratum contributes $(4\pi t)^{-1}\sum_{\ell=0}^\infty a_\ell^{(\mathcal{O})}t^\ell$ to this expansion (where $a_k^{(\mathcal{O})}$ are the integrals over $\mathcal{O}$ of certain curvature invariants, the same as in the case of manifolds), and any singular stratum $N \subset \mathcal{O}$ adds a contribution of the form

$$(4\pi t)^{-\dim(N)/2}\sum_{\ell=0}^{\infty} a_\ell^{(N)}t^\ell\,;$$

see [9, Theorem 4.8]. In the case $N = \{\overline{p}\}$, where $\overline{p} \in \mathcal{O}$ is a cone point of order $k \in \mathbb{N}$, arising from a rotation Φ with angle $\varphi := 2\pi/k$, one has $\dim(N) = 0$ and

$$a_\ell^{(\{\overline{p}\})} = \frac{1}{k}\sum_{j=1}^{k-1} b_\ell(\Phi^j), \tag{4.1}$$

where the b_ℓ are as in 3.1 (see [9, 4.5–4.8 & Example 5.3]). More precisely, the role of the manifold M of 3.1 is played here by the domain $\widetilde{U}$ of a local orbifold chart around $\overline{p}$, endowed with the pull-back of the Riemannian metric g (again denoted g), such that $(\widetilde{U}, g)/\{\mathrm{Id}, \Phi, \dots, \Phi^{k-1}\}$ is isometric to a neighborhood of p in $\mathcal{O}$; the point p of 3.1 is the preimage of $\overline{p}$.

Theorem 4.1. — *Let $\overline{p} \in (\mathcal{O}, g)$ be a cone point of order $k \in \mathbb{N}$ as above. Then*

$$\begin{aligned} a_2^{(\{\overline{p}\})} = {} & \left[\frac{1}{2520}\left(k^5 - \frac{1}{k}\right) + \frac{1}{720}\left(k^3 - \frac{1}{k}\right) + \frac{1}{180}\left(k - \frac{1}{k}\right)\right] K(\overline{p})^2 \\ & - \left[\frac{1}{15120}\left(k^5 - \frac{1}{k}\right) + \frac{1}{1440}\left(k^3 - \frac{1}{k}\right) + \frac{1}{180}\left(k - \frac{1}{k}\right)\right] \Delta_g K(\overline{p}). \end{aligned}$$

Proof. — Let p denote the preimage of $\overline{p}$ in an orbifold chart $(\widetilde{U}, g)$ as above. Note that with $\varphi := 2\pi/k$ and $C := \sqrt{2 - 2\cos\varphi}$ one has

$$C^2 = 4\sin^2\frac{\varphi}{2},$$

and by [7, p. 148] or, e.g., [18, 3.55],

$$\begin{aligned} \sum_{j=1}^{k-1}\frac{1}{\sin^4(j\cdot\frac{\pi}{k})} &= \frac{1}{45}(k^4-1) + \frac{2}{9}(k^2-1), \\ \sum_{j=1}^{k-1}\frac{1}{\sin^6(j\cdot\frac{\pi}{k})} &= \frac{2}{945}(k^6-1) + \frac{1}{45}(k^4-1) + \frac{8}{45}(k^2-1). \end{aligned}$$

Combining this with (4.1) and Theorem 3.7, we obtain

$$\begin{aligned}
&a_2^{(\{\bar{p}\})}\\
&= \frac{1}{k}\sum_{j=1}^{k-1}\left[\left(\frac{12}{4^3\sin^6(j\cdot\frac{\pi}{k})}-\frac{2}{4^2\sin^4(j\cdot\frac{\pi}{k})}\right)K(p)^2-\frac{2}{4^3\sin^6(j\cdot\frac{\pi}{k})}\Delta_g K(p)\right]\\
&= \frac{1}{k}\left\{\left[\frac{12\cdot 2}{64\cdot 945}(k^6-1)+\left(\frac{12\cdot 1}{64\cdot 45}-\frac{2\cdot 1}{16\cdot 45}\right)(k^4-1)\right.\right.\\
&\qquad\qquad\left.+\left(\frac{12\cdot 8}{64\cdot 45}-\frac{2\cdot 2}{16\cdot 9}\right)(k^2-1)\right]K(p)^2\\
&\qquad\left.-\left[\frac{2\cdot 2}{64\cdot 945}(k^6-1)+\frac{2\cdot 1}{64\cdot 45}(k^4-1)+\frac{2\cdot 8}{64\cdot 45}(k^2-1)\right]\Delta_g K(p)\right\}\\
&= \left[\frac{1}{2520}\left(k^5-\frac{1}{k}\right)+\frac{1}{720}\left(k^3-\frac{1}{k}\right)+\frac{1}{180}\left(k-\frac{1}{k}\right)\right]K(p)^2\\
&\qquad-\left[\frac{1}{15120}\left(k^5-\frac{1}{k}\right)+\frac{1}{1440}\left(k^3-\frac{1}{k}\right)+\frac{1}{180}\left(k-\frac{1}{k}\right)\right]\Delta_g K(p).
\end{aligned}$$

Finally, note that by definition of the curvature and the Laplacian on Riemannian orbifolds, $K(\overline{p}) = K(p)$ and $\Delta_g K(\overline{p}) = \Delta_g K(p)$. The theorem now follows. □

Remark 4.2. — Analogously, one could derive that

$$\begin{aligned}
a_0^{(\{\bar{p}\})} &= \frac{1}{12}\left(k-\frac{1}{k}\right),\\
a_1^{(\{\bar{p}\})} &= \left[\frac{1}{360}\left(k^3-\frac{1}{k}\right)+\frac{1}{36}\left(k-\frac{1}{k}\right)\right]K(\overline{p}),
\end{aligned}$$

for an orbisurface cone point $\overline{p}\in(\mathcal{O},g)$ of order k, using

$$\sum_{j=1}^{k-1}\frac{1}{\sin^2(j\cdot\pi/k)} = \frac{1}{3}(k^2-1) \quad\text{and}\quad b_0(\Phi)=\frac{1}{C}\,,\quad b_1(\Phi)=\frac{2}{C^2}K(p).$$

Note that the above formulas for $a_0^{(\{\bar{p}\})}$ and $a_1^{(\{\bar{p}\})}$ were already computed in [9, 5.6].

5. Corner contributions to the heat coefficients of geodesic polygons, up to degree two

In this section we follow ideas from [18, Section 4.3], concerning the case of interior angles of the form $\gamma = \pi/k$ in geodesic polygons. However, we drop the assumption of constant Gauss curvature which was present there and replace it by certain milder symmetricity assumptions (see (5.1) below).

Notation 5.1. — We consider a two-dimensional Riemannian manifold (M,g) again. Let P be a compact geodesic polygon in (M,g), and let $p \in M$ be one of its corners. Let γ be the interior angle of P at p. (For simplicity we assume that there is only one interior angle of P at the corner p, although more general settings as considered in [18] could be treated analogously.) As in 3.1, choose $\varepsilon_1 > 0$ such that $\exp_p|_{B_{\varepsilon_1}(0_p)}$ is a diffeomorphism onto its image

$$B := B_{\varepsilon_1}(p).$$

We now also assume that ε_1 is so small that $B \cap P$ is the image, under $\exp_p|_{B_{\varepsilon_1}(0_p)}$, of a circular sector of radius ε_1 in T_pM. Let E_0, E_1 be the two geodesic segments in $B \cap \partial P$ which meet at p, and let $u_0, u_1 \in S^1_p$ be unit vectors pointing into the direction of E_0 and E_1, respectively. Choose the orientation on B such that the rotation $D^\gamma : T_pM \to T_pM$ maps u_0 to u_1. Let $S : T_pM \to T_pM$ denote the reflection across $\mathbb{R}u_0$. We consider the diffeomorphisms

$$\sigma := \exp_p \circ S \circ \left(\exp_p|_{B_{\varepsilon_1}(0_p)}\right)^{-1} : B \to B,$$
$$\delta^\gamma := \exp_p \circ D^\gamma \circ \left(\exp_p|_{B_{\varepsilon_1}(0_p)}\right)^{-1} : B \to B.$$

Denote by G the group of diffeomorphisms of B generated by δ^γ and σ. We now assume that γ is of the form

$\gamma = \pi/k$ for some $k \geqslant 2$ in $\mathbb{N}$, so G is a dihedral group of order $4k$.

Moreover, we assume that, after possibly making ε_1 smaller,

$$G = \langle\{\delta^\gamma, \sigma\}\rangle \subset \mathrm{Isom}(B,g). \tag{5.1}$$

Note that G consists of the $2k$ rotations $\delta^{i\gamma} := (\delta^\gamma)^i$ with $i \in \{0,\dots,2k-1\}$ and the $2k$ reflections $\delta^{i\gamma} \circ \sigma$. (A special case in which the above symmetry assumptions hold is the case of B being a rotational surface with vertex p.) We choose $\varepsilon > 0$ such that $\varepsilon_2 := 2\varepsilon < \varepsilon_1$ and write

$$V := B_{2\varepsilon}(p) \subset B, \qquad U := B_\varepsilon(p) \subset V,$$
$$W_{2\varepsilon} := V \cap P, \qquad W_\varepsilon := U \cap P.$$

Finally, we denote by H_P, H_V, $H_{W_{2\varepsilon}}$ the Dirichlet heat kernels of P, V, and $W_{2\varepsilon}$, respectively.

Remark 5.2. — Let the situation be as above in 5.1, and let

$$Z_{W_\varepsilon}(t) := \int_{W_\varepsilon} H_P(t,q,q)\,\mathrm{d}q,$$

where $\mathrm{d}q$ abbreviates $\mathrm{dvol}_g(q)$. Note that the contribution of the interior angle at the corner p to the asymptotic expansion of the heat trace $t \mapsto \int_P H_P(t,q,q)\,\mathrm{d}q$ of P is the same as its contribution to the asymptotic expansion of the function Z_{W_ε} as just defined. We will now show, using the symmetry assumption (5.1), that the contribution of the interior angle $\gamma = \pi/k$ at p to the asymptotic expansion of $Z_{W_\varepsilon}(t)$ equals $\frac{1}{2}$ times the contribution of a cone point $\overline{p}$ of order k to the heat kernel coefficients of a Riemannian orbisurface, where $\overline{p}$ has a neighborhood isometric to B divided by a group of rotations about p. One could show this by using arguments analogous to those in [18, p. 142–144]. We choose a related, but slightly different argument using a little trick (see (5.3) below) involving rotations, as in the computation in [18, p. 108].

First of all, by the Principle of not feeling the boundary (recall Remark 3.3 (i)), we can replace $H_P(t,q,q)$ by $H_{W_{2\varepsilon}}(t,q,q)$ in the definition of $Z_{W_\varepsilon}(t)$ without changing its asymptotic expansion as $t \searrow 0$. Next, we describe $H_{W_{2\varepsilon}}(t,q,q)$ using Sommerfeld's method of images (see also [18, Section 3.4]): For $i \in \{0,\dots,2k-1\}$ let

$$\sigma_i := \delta^{i\gamma} \circ \sigma \circ \delta^{-i\gamma} \in \mathrm{Isom}(B,g)$$

denote the reflection across the geodesic with initial vector $(D^\gamma)^i(u_0) = D^{i\gamma}(u_0)$. Of course, $\sigma_i = \sigma_{i+k}$ for $i \in \{0,\dots,k-1\}$. Write

$$\Psi_i := \sigma_i \circ \cdots \circ \sigma_1 \text{ for } i \in \{1,\dots,2k-1\}, \quad \text{and} \quad \Psi_0 := \mathrm{Id}_V\,.$$

Then

$$H_{W_{2\varepsilon}}(t,q,q) = \sum_{i=0}^{2k-1} (-1)^i H_V(t,q,\Psi_i(q))$$

for all $t > 0$ and $q \in W$. So the small-time asymptotic expansion of $Z_{W_\varepsilon}(t)$ is the same as that of

$$\sum_{i=0}^{2k-1} (-1)^i \int_{W_\varepsilon} H_V(t,q,\Psi_i(q))\,\mathrm{d}q. \tag{5.2}$$

We now show that sum of those summands which correspond to odd indices i does actually not enter into the corner contribution: Note that

$\Psi_{2j-1} = \sigma_j$ for $j \in \{1, \dots, k\}$ and thus, using $\sigma_j = \delta^{j\gamma} \circ \sigma_0 \circ \delta^{-j\gamma}$:

$$\begin{aligned}(5.3)\quad \sum_{j=1}^{k} \int_{W_\varepsilon} (-1)^{2j-1} H_V(t, q, \Psi_{2j-1}(q))\,\mathrm{d}q \\ &= -\sum_{j=1}^{k} \int_{W_\varepsilon} H_V(t, \delta^{-j\gamma} q, \delta^{-j\gamma} \sigma_j(q))\,\mathrm{d}q \\ &= -\sum_{j=1}^{k} \int_{W_\varepsilon} H_V(t, \delta^{-j\gamma} q, \sigma_0(\delta^{-j\gamma}(q))\,\mathrm{d}q \\ &= -\sum_{j=1}^{k} \int_{\delta^{-j\gamma}(W_\varepsilon)} H_V(t, q, \sigma_0(q))\,\mathrm{d}q \\ &= -\int_{\bigcup_{j=1,\dots,k} \delta^{-j\gamma}(W_\varepsilon)} H_V(t, q, \sigma_0(q))\,\mathrm{d}q \\ &= -\int_{U'} H_V(t, q, \sigma_0(q))\,\mathrm{d}q,\end{aligned}$$

where $U' := \bigcup_{j=1,\dots,k} \delta^{-j\gamma}(W_\varepsilon)$ is a half-disc; U' is that part of $U = B_\varepsilon(p)$ that lies on the same side of $L_\varepsilon := \exp_p(\{ru_0 \mid r \in (-\varepsilon, \varepsilon)\})$ as $\sigma_0(W_\varepsilon) = \delta^{-\gamma}(W_\varepsilon)$. In particular, U' has no corner at p, and the small-time asymptotic expansion of (5.3) will yield only the contribution of the straight boundary segment L_ε to the Dirichlet heat trace expansion of the analogous half-disc $V' \subset V$.

Write $\varphi := 2\gamma = 2\pi/k$ and $\Phi := \delta^\varphi$. Then, on the other hand, the sum of those summands in (5.2) which correspond to even indices i gives, using $\Psi_{2j} = \delta^{2j\gamma}$ and the symmetry condition (5.1):

$$\begin{aligned}\sum_{j=0}^{k-1} \int_{W_\varepsilon} (-1)^{2j} H_V(t, q, \Psi_{2j}(q))\,\mathrm{d}q &= \frac{1}{2} \cdot 2 \sum_{j=0}^{k-1} \int_{W_\varepsilon} H_V(t, q, \delta^{2j\gamma}(q))\,\mathrm{d}q \\ = \frac{1}{2} \sum_{j=0}^{k-1} \int_{W_\varepsilon \cup \delta^\gamma(W_\varepsilon)} H_V(t, q, \delta^{2j\gamma}(q))\,\mathrm{d}q &= \frac{1}{2k} \sum_{j=0}^{k-1} \int_{U} H_V(t, q, \Phi^j(q))\,\mathrm{d}q.\end{aligned}$$

By (3.1), the asymptotic expansion for $t \searrow 0$ of this sum is

$$\frac{1}{2k} \sum_{j=0}^{k-1} \sum_{\ell=0}^{\infty} b_\ell(\Phi^j) t^\ell = \sum_{\ell=0}^{\infty} \alpha_\ell t^\ell \quad \text{with} \quad \alpha_\ell := \frac{1}{2k} \sum_{j=0}^{k-1} b_\ell(\Phi_j).$$

By (4.1), we have $\alpha_\ell = \frac{1}{2} a_\ell^{(\{\bar{p}\})}$, where $\bar{p}$ is a cone point of order k in any closed orbisurface $\mathcal{O}$ with the property that some neighborhood of $\bar{p}$

is isometric to $B/\{\Phi^j \mid j=0,\dots,k-1\}$. We know the values of $\frac{1}{2}a_0^{(\{\bar p\})}$, $\frac{1}{2}a_1^{(\{\bar p\})}$, $\frac{1}{2}a_2^{(\{\bar p\})}$ from Remark 4.2 and Theorem 4.1. Finally, note that

$$k^{m-1}-\frac{1}{k}=\frac{\pi^m-\gamma^m}{\gamma^{m-1}\pi}$$

since $\gamma=\pi/k$. So we have shown:

Main Theorem 5.3. — *In the situation of Notation 5.1, with the symmetry assumption* (5.1)*, the contribution of the corner p with interior angle $\gamma=\pi/k$ (where $k\in\mathbb{N}$, $k\geqslant 2$) to the asymptotic expansion of the heat trace associated with the Dirichlet Laplacian of the geodesic polygon P has the form $\sum_{\ell=0}^{\infty}c_\ell(\gamma)t^\ell$ with the coefficients $c_\ell(\gamma)$ given by*

$$c_\ell(\gamma)=\frac{1}{2}a_\ell^{(\{\bar p\})},$$

where $\bar p$ is an orbisurface cone point of order k having a neighborhood isometric to $B/\{\delta^{2j\gamma}\mid j=0,\dots,k-1\}$. In particular, by Theorem 4.1,

$$c_0(\gamma)=\frac{\pi^2-\gamma^2}{24\gamma\pi}, \tag{5.4}$$

$$c_1(\gamma)=\left(\frac{\pi^4-\gamma^4}{720\gamma^2\pi}+\frac{\pi^2-\gamma^2}{72\gamma\pi}\right)K(p), \tag{5.5}$$

$$\begin{aligned}c_2(\gamma)=&\left(\frac{\pi^6-\gamma^6}{5040\gamma^5\pi}+\frac{\pi^4-\gamma^4}{1440\gamma^3\pi}+\frac{\pi^2-\gamma^2}{360\gamma\pi}\right)K(p)^2\\&-\left(\frac{\pi^6-\gamma^6}{30240\gamma^5\pi}+\frac{\pi^4-\gamma^4}{2880\gamma^3\pi}+\frac{\pi^2-\gamma^2}{360\gamma\pi}\right)\Delta_g K(p).\end{aligned} \tag{5.6}$$

(As always in this article, Δ_g here denotes $-\operatorname{div}_g\circ\operatorname{grad}_g$.)

Remarks 5.4.

(i) Formula (5.4) for $c_0(\gamma)$ seems well-known, even for general γ (not only those of the form $\gamma=\pi/k$) and without any symmetry assumptions; see, e.g., the discussion in [13]. Of course, in the case of euclidean polygons this is obvious from the classical formula (1.1) found by D. Ray and proved by van den Berg and Srisatkunarajah [1].

(ii) In the case of constant curvature $K=1$, the above formulas (5.4), (5.5), (5.6) (even for general $\gamma\in(0,2\pi]$) were proved by Watson [19]. In the case of arbitrary constant curvature $K\in\mathbb{R}$ the same was proved by Uçar in [18], the main breakthrough there being the computation of the Green kernel for an arbitrary geodesic wedge in the hyperbolic plane. Those authors actually computed $c_\ell(\gamma)$ for *every* $\ell\in\mathbb{N}_0$ in the case $K=1$, resp. $K\in\mathbb{R}$ constant. It turns out that for constant curvature K, one has $c_\ell(\gamma) = f_\ell(\gamma) \cdot K^\ell$ for certain rational functions f_ℓ. Of course, based on Uçar's and Watson's formulas, the above formula for $c_1(\gamma)$, as well as the coefficient at $K(p)^2$ in $c_2(\gamma)$, was to be expected. However, the constant curvature case did not provide insight into the way in which $\Delta_g K(p)$ (which is, up to linear combinations, the only other curvature invariant of order four in dimension two besides $K(p)^2$) might enter into $c_2(\gamma)$.

(iii) To the author's best knowledge, formula (5.6) for $c_2(\gamma)$ (with $\gamma \in \{\pi/k \mid k \in \mathbb{N}\}$ and under the symmetry assumptions (5.1)), especially its coefficient at $\Delta_g K(p)$, was not known previously. In particular, the main theoretic insight that this formula provides is that here the coefficient at $\Delta_g K(p)$ is a rational function of γ, and that it is of a similar structure as the coefficient at $K(p)^2$. We expect that the formula extends to general $\gamma \in (0, 2\pi]$; see Conjecture 5.5. below.

(iv) Note that the symmetry condition (5.1), which has been necessary for our approach, implies that the gradient of K at p vanishes. Therefore, the methods of the present article cannot lead in any way, in situations where that symmetry condition is absent, to any knowledge about the possible coefficient of $\|\nabla K(p)\|^2$ in $c_3(\gamma)$ (note that $\|\nabla K(p)\|^2$ is one of the curvature invariants of order six). Concerning $c_2(\gamma)$, however, we expect that formula (5.6) from the above theorem holds more generally, at least if $\nabla^2 K_p$ still is a multiple of g_p. So we conclude this paper with the following conjecture:

Conjecture 5.5. — *Let $\gamma \in (0, 2\pi]$, and let P be a compact geodesic polygon in a two-dimensional Riemannian manifold (M, g). Let p be a corner of P with interior angle $\gamma \in (0, 2\pi]$, and assume that $\nabla^2 K_p$ is a multiple of g_p. Then the coefficient at t^2 in the small-time asymptotic expansion of the Dirichlet heat kernel of P is given by formula* (5.6).

Appendix A. Proof of Lemma 2.3

We partly follow Nicolaescu's approach from [16, Appendix A]. He considered Riemannian manifolds of arbitrary dimension n and there derived the expansion of $\mathrm{dist}(\exp_p(x), \exp_p(y))$ up to order four. In dimension two, his formula corresponds to the first two terms of formula (2.8), with $K(p)\|x \wedge y\|^2$ replaced by $\langle R(x, y)y, x\rangle$. The idea in [16] is to use the fact that for any $q \in M$, the function $f := \mathrm{dist}^2(q, \cdot\,) : M \to \mathbb{R}$ satisfies, wherever it is smooth (in particular, near q), a so-called Hamilton–Jacobi equation:

$$\|\mathrm{d}f\|^2 = 4f. \tag{A.1}$$

Here we use $\|\cdot\|$ to denote the pointwise norm canonically induced by g on tensor fields, and we will do similarly for $\langle\,\cdot\,,\cdot\,\rangle$.

Choose a small neighborhood W of $0 \in T_pM$ contained in the domain of injectivity of $\exp_p$ and such that $U := \exp_p(W) \subset M$ is convex (meaning that for all $q, w \in U$, there exists a unique geodesic in M with length $\mathrm{dist}(q, w)$, and that geodesic is contained in U). Consider

$$F : W \times W \ni (x, y) \mapsto \mathrm{dist}^2(\exp_p(x), \exp_p(y)) \in \mathbb{R}.$$

We write the Taylor expansion of F at $(0, 0)$ in the form

$$\begin{gathered}(T^\infty_{(0,0)}F)(x, y) = (F_0 + F_1 + F_2 + F_3 + \ldots)(x, y)\\ \text{with } F_m = F_{m,0} + F_{m-1,1} + \ldots + F_{0,m}\,,\end{gathered} \tag{A.2}$$

where each $F_{k,\ell}(x, y)$ is k-linear in x and ℓ-linear in y. Since F is symmetric, $F_{\ell,k}$ is obtained from $F_{k,\ell}$ by interchanging x and y. Moreover,

$$F(x, 0) = \|x\|^2, \quad \text{hence } F_{k,0} = 0 = F_{0,k} \text{ for all } k > 2.$$

Note that by the First Variation Formula we have

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} F(tx, y) = -2\langle x, y\rangle, \quad \text{hence } F_{1,k} = 0 = F_{k,1} \text{ for all } k > 1.$$

(This was not used in [16].) In particular,

$$F_3 = 0 \;\text{ and }\; F_4 = F_{2,2}$$

(as already known), and what we are actually after are explicit formulas, in our two-dimensional setting, for

$$F_5 = F_{3,2} + F_{2,3} \;\text{ and }\; F_6 = F_{4,2} + F_{3,3} + F_{2,4}.$$

For each $y \in W$, $F^y := F(\,\cdot\,, y) : W \to \mathbb{R}$ is smooth. Let $\hat{g}$ be the Riemannian metric $(\exp_p|_W)^*g$ on W. Then (A.1) says

$$4F^y = \|\mathrm{d}F^y\|^2_{\hat{g}}.$$

Since we assume $\dim M = 2$, we can express $\|(\mathrm{d}F^y)_x\|^2_{\hat{g}}$ at each nonzero $x \in W$ as follows: Consider the $\hat{g}$-orthonormal basis $\{x/\|x\|, \widetilde{x}/\|\widetilde{x}\|_{\hat{g}}\}$ of

T_xW, where $\widetilde{x} \in T_xW$ denotes the 90-degree rotation of x with respect to an arbitrarily chosen orientation on the euclidean plane (T_pM, g_p). Then

$$\begin{aligned} \|(\mathrm{d}F^y)_x\|^2_{\hat{g}} &= (\mathrm{d}F^y)_x(x)^2/\|x\|^2 + (\mathrm{d}F^y)_x(\widetilde{x})^2/\|\widetilde{x}\|^2_{\hat{g}} \\ &= \left((\mathrm{d}F^y)_x(x)^2 + (\mathrm{d}F_y)_x(\widetilde{x})^2\right)/\|x\|^2 - (\mathrm{d}F^y)_x(\widetilde{x})^2/\|x\|^2 \\ &\qquad + (\mathrm{d}F^y)_x(\widetilde{x})^2/\|\widetilde{x}\|^2_{\hat{g}} \\ &= \|(\mathrm{d}F^y)_x\|^2 + (\mathrm{d}F^y)_x(\widetilde{x})^2(\|\widetilde{x}\|^{-2}_{\hat{g}} - \|x\|^{-2}) \end{aligned} \tag{A.3}$$

For this, recall that $\|\cdot\|$ denotes the norm with respect to g_p, and for x viewed as an element of T_xW, $\|x\|_{\hat{g}} = \|x\|$ since $\exp_p$ is a radial isometry. Using (2.2) for $u = x/\|x\|$, $r = \|x\|$ and noting that

$$\|(\mathrm{d}\exp_p)_x(\widetilde{x})\| = \theta_u(r)\|\widetilde{x}\| = \theta_u(r)\|x\|,$$

we have, for $\widetilde{x}$ viewed as an element of T_xW:

$$\begin{aligned} \|\widetilde{x}\|_{\hat{g}} = \|x\| - \frac{1}{6}K(p)\|x\|^3 - \frac{1}{12}\mathrm{d}K_p(x)\|x\|^3 + \frac{1}{120}K(p)^2\|x\|^5 \\ - \frac{1}{40}\nabla^2 K_p(x,x)\|x\|^3 + O(\|x\|^6). \end{aligned}$$

By the resulting expansion of $\|\widetilde{x}\|^{-2}_{\hat{g}}$ and (A.3), equation (A.1) becomes

$$\begin{aligned} 4F(x,y) = \|(\mathrm{d}F^y)_x\|^2 + (\mathrm{d}F^y)_x(\widetilde{x})^2 \cdot \Bigg(\frac{1}{3}K(p) + \frac{1}{6}\mathrm{d}K_p(x) \\ + \frac{1}{15}K(p)^2\|x\|^2 + \frac{1}{20}\nabla^2 K_p(x,x) + O(\|x\|^3)\Bigg). \end{aligned}$$

Comparing the terms of total order five in x and y in this equation we get, writing $F_m^y := F_m(\,\cdot\,, y)$, noting that $(\mathrm{d}F_m^y)_x$ is of total order $m-1$, and recalling $F_0 = 0$, $F_1 = 0$, $F_2(x,y) = \|x-y\|^2$, $F_3 = 0$:

$$\begin{aligned} 4F_5(x,y) &= 2\langle(\mathrm{d}F_5^y)_x, (\mathrm{d}F_2^y)_x\rangle + (\mathrm{d}F_2^y)_x(\widetilde{x})^2 \cdot \frac{1}{6}\mathrm{d}K_p(x) \\ &= 4(\mathrm{d}F_5^y)_x(x-y) + 4\langle x-y, \widetilde{x}\rangle^2 \cdot \frac{1}{6}\mathrm{d}K_p(x). \end{aligned}$$

In particular, by $(\mathrm{d}F_{k,\ell}^y)_x(x) = kF_{k,\ell}(x,y)$ we have

$$4F_{3,2}(x,y) = 12F_{3,2}(x,y) + 4\|x \wedge y\|^2 \cdot \frac{1}{6}\mathrm{d}K_p(x),$$

which gives

$$F_{3,2}(x,y) = -\frac{1}{12}\mathrm{d}K_p(x)\|x \wedge y\|^2.$$

The claimed form of F_5 now follows by symmetry in x and y. Similarly, taking the well-known formula

$$F_4(x,y) = -\frac{1}{3}K(p)\|x\wedge y\|^2$$

for granted (which could otherwise first been proved analogously), and using

$$\begin{aligned}(\mathrm{d}F_2^y)_x(\widetilde{x}) &= -2\langle\widetilde{x},y\rangle,\\ (\mathrm{d}F_4^y)_x(\widetilde{x}) &= \frac{2}{3}K(p)\langle x,y\rangle\langle\widetilde{x},y\rangle,\\ \langle\widetilde{x},y\rangle^2 &= \|x\wedge y\|^2,\end{aligned}$$

we obtain

$$\begin{aligned}4F_6(x,y) &= \|(\mathrm{d}F_4^y)_x\|^2 + 2\langle(\mathrm{d}F_6^y)_x,(\mathrm{d}F_2^y)_x\rangle\\ &\qquad + 2(\mathrm{d}F_2^y)_x(\widetilde{x})(\mathrm{d}F_4^y)_x(\widetilde{x})\cdot\frac{1}{3}K(p)\\ &\qquad + (\mathrm{d}F_2^y)_x(\widetilde{x})^2\cdot\left(\frac{1}{15}K(p)^2\|x\|^2+\frac{1}{20}\nabla^2K_p(x,x)\right)\\ &= \frac{4}{9}K(p)^2\|x\wedge y\|^2\|y\|^2 + 4(\mathrm{d}F_6^y)_x(x-y)\\ &\qquad - \frac{8}{9}K(p)^2\|x\wedge y\|^2\langle x,y\rangle\\ &\qquad + 4\|x\wedge y\|^2\cdot\left(\frac{1}{15}K(p)^2\|x\|^2+\frac{1}{20}\nabla^2K_p(x,x)\right).\end{aligned}$$

In particular,

$$4F_{4,2}(x,y) = 16F_{4,2}(x,y) + 4\|x\wedge y\|^2\cdot\left(\frac{1}{15}K(p)^2\|x\|^2+\frac{1}{20}\nabla^2K_p(x,x)\right).$$

Thus,

$$F_{4,2}(x,y) = \|x\wedge y\|^2\cdot\left(-\frac{1}{45}K(p)^2\|x\|^2-\frac{1}{60}\nabla^2K_p(x,x)\right),$$

and the analogous expression for $F_{2,4}(x,y)$, as claimed. Finally,

$$\begin{aligned}4F_{3,3}(x,y) &= 4(\mathrm{d}F_{4,2}^y)_x(-y) + 4(\mathrm{d}F_{3,3}^y)_x(x) - \frac{8}{9}K(p)^2\|x\wedge y\|^2\langle x,y\rangle\\ &= \|x\wedge y\|^2\cdot\left(\frac{8}{45}K(p)^2\langle x,y\rangle+\frac{8}{60}\nabla^2K_p(x,y)\right) + 12F_{3,3}(x,y)\\ &\qquad - \frac{8}{9}K(p)^2\|x\wedge y\|^2\langle x,y\rangle,\end{aligned}$$

yielding

$$F_{3,3}(x,y) = \|x \wedge y\|^2 \cdot \left(\frac{4}{45} K(p)^2 \langle x,y \rangle - \frac{1}{60} \nabla^2 K_p(x,y) \right),$$

as claimed.

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