ROCKY MOUNTAIN
JOURNAL OF MATHEMATICS
Volume 48, Number 3, 2018

SEMIGROUP ASYMPTOTICS, THE FUNK-HECKE IDENTITY AND THE GEGENBAUER COEFFICIENTS ASSOCIATED WITH THE SPHERICAL LAPLACIAN

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ABSTRACT. A trace formulation of the Maclaurin spectral coefficients of the Schwartzian kernel of functions of the spherical Laplacian is given. A class of polynomials $\mathscr{P}_l^\nu(X)$ ($l \geq 0$, $\nu > -1/2$) linking to the classical Gegenbauer polynomials through a differential-spectral identity is introduced, and its connection to the above spectral coefficients and their asymptotics analyzed. The paper discusses some applications of these ideas combined with the Funk-Hecke identity and semigroup techniques to geometric and variational-energy inequalities on the sphere and presents some examples.

1. Introduction. Let $(\mathscr{X}, g)$ be a smooth compact n-dimensional Riemannian manifold without boundary, and let $\Delta = \Delta_g$ denote the Laplace-Beltrami operator on $\mathscr{X}$ given in local coordinates via

$$\Delta_g = \frac{1}{\sqrt{\det g}} \sum_{j=1}^{n} \partial_j \bigg(\sum_{k=1}^{n} \sqrt{\det g}\, g^{jk} \partial_k \bigg).$$

By basic spectral theory, there exists a complete orthonormal basis $(\varphi_k : k \geq 0)$ of eigenfunctions of $-\Delta_g$ in $L^2(\mathscr{X}, dv_g)$ with the associated eigenvalues $(\lambda_k : k \geq 0)$ verifying $-\Delta_g \varphi_k = \lambda_k \varphi_k$. Each λ_k has finite multiplicity, and the spectrum $\Sigma(-\Delta_g)$ can be arranged in ascending order $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$ with $\lambda_j \nearrow \infty$. Moreover, by orthogonality, $(\varphi_j, \varphi_k)_{L^2(\mathscr{X})} = 0$ for $0 \leq j \neq k$ whilst $\|\varphi_j\|_{L^2(\mathscr{X})} = 1$ for all $j \geq 0$ by suitable normalization.

Now, for a given function $\Phi = \Phi(X)$ in the Borel functional calculus of $-\Delta_g$, the Schwartzian (or integral) kernel of the operator $\Phi(-\Delta_g)$

2010 AMS *Mathematics subject classification.* Primary 47B25, 47F05, Secondary 33C05, 33C20, 33C45, 47D06, 47E05, 58J35.

Keywords and phrases. Gegenbauer polynomials, Laplace-Beltrami operator, Funk-Hecke identity, Maclaurin spectral coefficients, energy inequalities.

Received by the editors on July 7, 2017.

DOI:10.1216/RMJ-2018-48-3-791

can be expressed by the spectral sum $\sum \Phi(\lambda_k)\,\varphi_k \otimes \varphi_k$, or more specifically, by the sum

$$K_\Phi(x,y) = \sum_{k=0}^{\infty} \Phi(\lambda_k)\varphi_k(x)\varphi_k(y), \quad x,y \in \mathscr{X}. \tag{1.1}$$

In the case of the heat semigroup with $\Phi(X) = e^{-tX}$ $(t > 0)$ the analysis of the heat kernel and its asymptotics has been the subject of numerous fruitful investigations in the past 60 years, leading to some profound and deep results whose scope of applications range from direct and inverse spectral theory, index theory, number theory and automorphic forms to quantum field theory, and many more. For instance, the short time asymptotics of the heat kernel of a compact Riemannian manifold as first studied and formulated by Minakshisundaram and Pleijel **[24]** through the construction of the so-called heat parametrix (more details follow) has resulted, by application of suitable Tauberian theorems, in a precise formulation of the leading term in Weyl's law, as well as a complete description of the poles and residues of the spectral zeta function $\zeta_{\mathscr{X}} = \zeta_{\mathscr{X}}(s)$ on $\mathscr{X}$ (see **[7, 13, 34]** and the references therein). As the heat semigroup is of trace class, it has a well-defined and finite-valued trace whose short time asymptotics ($t \searrow 0$) takes the form **[24]** (cf., also, **[7, 13]**)

$$\operatorname{tr} T(t) = \operatorname{tr} e^{t\Delta_g} = \int_{\mathscr{X}} K_t(x,x)\, dv_g(x) = \sum_{k=0}^{\infty} e^{-\lambda_k t} \sim \sum_{k=0}^{\infty} \frac{a_k^n(\mathscr{X}) t^k}{(4\pi t)^{n/2}}. \tag{1.2}$$

The sequence of scalars $(a_k^n : k \geq 0)$, called the *heat coefficients* or the *heat invariants* (also known as the Minakshisundaram-Pleijel heat coefficients), associated with $(\mathscr{X}, g)$ are geometric invariants that can be entirely described through the Riemann curvature tensor R and its successive covariant derivatives. For instance, the leading coefficient a_0^n is always the volume $\mathrm{Vol}_g(\mathscr{X})$, a_1^n is a constant multiple of the total scalar curvature (see below) and the further terms become increasingly more complicated integrals of polynomial expressions in R and its derivatives (see, e.g., **[7, 8, 12, 13, 21, 29]** for further details on heat coefficients and local heat invariants, and, for some deep and far reaching implications, see **[10, 11, 17, 23, 28, 31, 32]**). In particular, and as a consequence, the first few terms in the heat trace expansion

(1.2) can be written as ($t \searrow 0$)

$$\Theta(t) = \operatorname{tr} T(t) = \sum_{k=0}^{\infty} e^{-\lambda_k t}$$

$$\sim \frac{1}{(4\pi t)^{n/2}} \Big\{ \mathrm{Vol}_g(\mathscr{X}) + t \int_{\mathscr{X}} \frac{\mathrm{Scal}}{6}\, dv_g \tag{1.3}$$

$$+ t^2 \int_{\mathscr{X}} \frac{5\,\mathrm{Scal}^2 - 2|\mathrm{Ric}|^2 + 2|\mathrm{R}|^2}{360}\, dv_g + O(t^3) \Big\}$$

where R, Ric and Scal denote the Riemann curvature tensor, the Ricci curvature tensor and the scalar curvature of $(\mathscr{X}, g)$, and $|\mathrm{R}|$, $|\mathrm{Ric}|$ are the norms of R, Ric, respectively, **[21, 23]**.

In the case of a compact rank one symmetric space $\mathscr{X} = G/K$ of a compact Lie group G and with K the isotropy group of a point in $\mathscr{X}$, starting from the spectral sum (1.1) and using the addition formula for the matrix coefficients of the irreducible unitary representations, it can be seen that the Schwartzian kernel K_Φ of the invariant operator $\Phi(-\Delta)$ takes the form

$$K_\Phi(\theta) = \frac{1}{\mathrm{Vol}(\mathscr{X})} \sum_{k=0}^{\infty} M_k^n \Phi_k(\theta; \mathscr{X}) \Phi(\lambda_k^n), \tag{1.4}$$

where $\Phi_k = \Phi_k(\theta; \mathscr{X})$ are the spherical functions on $\mathscr{X}$, $\lambda_k^n = \lambda_k^n(\mathscr{X})$ are the numerically *distinct* eigenvalues of the Laplacian on $\mathscr{X}$, $M_k^n = M_k^n(\mathscr{X})$ is the dimension of the eigenspace associated with λ_k^n, $\theta = \theta(x, y)$ is the distance between the points $x, y \in \mathscr{X}$ and $\mathrm{Vol}(\mathscr{X})$ denotes the volume of $\mathscr{X}$. Specializing further to the n-sphere $\mathscr{X} = \mathbb{S}^n$ (note the identification $\mathbb{S}^n = \mathbf{SO}(n+1)/\mathbf{SO}(n)$) it is seen that the spherical or zonal functions here can be expressed via the *normalized* Gegenbauer polynomials (see Appendix A) as $\Phi_k = \mathscr{C}_k^\nu(\cos\theta)$ (with $\nu = (n-1)/2$) where, as eigenfunctions, $-\Delta\Phi_k = \lambda_k^n \Phi_k$ while $\Phi_k(0) = 1$ (cf., (A.4), (A.6)). Hence, (1.4) leads to

$$K_\Phi(\theta) = \sum_{k=0}^{\infty} \frac{(k+n-2)!}{\omega_n k!(n-1)!} (2k+n-1) \Phi(k(k+n-1)) \mathscr{C}_k^{(n-1)/2}(\cos\theta), \tag{1.5}$$

where $\lambda_k^n = k(k+n-1)$ with $k \geq 0$ are the distinct eigenvalues of $-\Delta$ on $\mathbb{S}^n$, $M_k^n = (2k+n-1)(k+n-2)!/(k!(n-1)!)$ is the multiplicity of λ_k^n, $\cos\theta = x \cdot y$ and $\omega_n = \mathrm{Vol}(\mathbb{S}^n) = 2\pi^{(n+1)/2}/\Gamma((n+1)/2)$. Now, in view of the Schwartzian kernel K_Φ being an even function, subject to sufficient regularity, it admits a formal Maclaurin expansion about the origin $\theta = 0$ as

$$\sum_{l=0}^{\infty} \frac{\partial^{2l}}{\partial\theta^{2l}} K_\Phi \Big|_{\theta=0} \frac{\theta^{2l}}{(2l)!} = \frac{1}{\omega_n} \sum_{l=0}^{\infty} \frac{b_{2l}^n}{(2l)!} \theta^{2l}. \tag{1.6}$$

The Maclaurin spectral coefficients $b_{2l}^n = b_{2l}^n[\Phi]$ can be explicitly described by invoking a spectral-differential identity on the normalized Gegenbauer polynomials, proven in Theorem 2.1 below. Indeed, it follows as an immediate result that $b_0^n = \operatorname{tr}\Phi(-\Delta)$, while, for $l \geq 1$, and with $\nu = (n-1)/2$,

(1.7)
$$b_{2l}^n = \omega_n \frac{\partial^{2l}}{\partial\theta^{2l}} K_\Phi \Big|_{\theta=0} = \sum_{k=0}^{\infty} M_k^n \Phi(\lambda_k^n) \sum_{j=1}^{l} \mathsf{c}_j^l [\lambda_k^n]^j = \operatorname{tr}[\Phi \mathscr{P}_l](-\Delta),$$

where $\mathscr{P}_l = \mathscr{P}_l^\nu(X)$ (with $l \geq 1$) is the degree l polynomial in X given explicitly by (2.3) below. The above identity and its variants, including a representation by Jacobi theta series, are further explored in Section 3. In Section 4, we study the asymptotics of the Maclaurin spectral coefficients through those of the heat invariants and theta series that, in particular, enable us to recover some associated and classical heat asymptotics. In Section 5, as a further application, we study semigroups generated by functions of the spherical Laplacian and a new class of geometric inequalities resulting from them. Here, with the aid of the Funk-Hecke identity, we are able to gain more insight into the nature of the associated Maclaurin spectral coefficients and the structure and form of the variational-energy inequalities. For more motivation and discussion including applications to kernel approximation, construction of continuous wavelets and others, see [**2, 4, 5, 14, 16, 20, 32, 34**] and the references therein.

2. The differential action $\mathsf{P}(d/d\theta)\mathscr{C}_k^\nu(\cos\theta)$ and the associated polynomials $\mathscr{P}_l^\nu = \mathscr{P}_l^\nu(X)$. Let $\mathsf{P} = \mathsf{P}_d(X)$ be a polynomial of degree $d \geq 2$ with a choice of coefficients $\mathsf{A}_0, \dots, \mathsf{A}_d$; specifically, $\mathsf{P}(X) = \sum \mathsf{A}_i X^i$, with $0 \leq i \leq d$, and the associated constant coefficient differential operator $\mathscr{L}$, defined formally by

$$\mathscr{L} = \mathsf{P}(d/d\theta) = \sum_{i=0}^{d} \mathsf{A}_i d^i/d\theta^i. \tag{2.1}$$

In the following, the differential operator $\mathscr{L}$ will be applied to the normalized Gegenbauer polynomials which then results in an interesting differential-spectral identity that motivates the introduction of a new scale of polynomials.

Theorem 2.1. *For $\mathscr{L} = \mathsf{P}(d/d\theta)$ as in* (2.1)*, the normalized Gegenbauer polynomial $\mathscr{C}_k^\nu$ with $k \geq 1$, $\nu > -1/2$, satisfies the identity*

$$\begin{aligned} \mathsf{P}(d/d\theta)\mathscr{C}_k^\nu(\cos\theta)\big|_{\theta=0} &= \mathsf{A}_0 + \sum_{l=1}^{[d/2]} \mathsf{A}_{2l} \sum_{j=1}^{l} \mathsf{c}_j^l(\nu)[\lambda_k^\nu]^j \\ &= \mathsf{A}_0 + \sum_{l=1}^{[d/2]} \mathsf{A}_{2l} \mathscr{P}_l^\nu(\lambda_k^\nu), \end{aligned} \tag{2.2}$$

where $\lambda_k^\nu = k(k+2\nu)$ are the eigenvalues of the Gegenbauer operator (A.4)*. Furthermore, the polynomial $\mathscr{P}_l^\nu = \mathscr{P}_l^\nu(X)$ and its coefficients $\mathsf{c}_j^m(\nu)$ are given by*

$$\begin{aligned} \mathscr{P}_l^\nu(X) &= \sum_{j=1}^{l} \mathsf{c}_j^l(\nu) X^j, \\ \mathsf{c}_j^l(\nu) &= \sum_{m=j}^{l} \frac{2^m \Gamma(\nu+m)\Gamma(2\nu)\mathsf{b}_j^m}{\Gamma(\nu)\Gamma(2\nu+2m)} \mathsf{B}_{2l,m}(\zeta), \end{aligned} \tag{2.3}$$

where b_j^m are defined recursively as: $\mathsf{b}_m^m = 1$, $\mathsf{b}_0^m = 0$ for $m \geq 1$ and $\mathsf{b}_j^{m+1} = \mathsf{b}_{j-1}^m - m(m+2\nu)\mathsf{b}_j^m$ for $1 \leq j \leq m$, $\mathsf{B}_{2l,m}$ are the Bell polynomials (*see the Appendix*)*, and $\zeta = (\zeta_k)$ is the sequence $\zeta_k = (-1)^{k/2}$ for k even and zero otherwise.*

Proof. Since $\mathscr{C}_k^\nu(\cos\theta)$ is an even function, all of its odd derivatives vanish at $\theta = 0$, and so we are left with the task of calculating only the even derivatives. Using Faà de Bruno's formula (B.3) and (B.1), we have

$$[d^{2l}C_k^\nu(\cos\theta)/d\theta^{2l}]\big|_{\theta=0} = \sum_{m=1}^{l}[d^mC_k^\nu(t)/dt^m]\big|_{t=1}\mathsf{B}_{2l,m}(\zeta)$$

for $l \geq 1$ and, invoking the recursive relation (A.3) (with $m \geq 1$), we have, for ζ, as expressed in the statement of the proposition,

$$\frac{d^{2l}}{d\theta^{2l}}C_k^\nu(\cos\theta)\big|_{\theta=0} = \sum_{m=1}^{l}\frac{\Gamma(\nu+m)}{2^{-m}\Gamma(\nu)}C_{k-m}^{\nu+m}(1)\mathsf{B}_{2l,m}(\zeta) = \sum_{m=1}^{l}\mathsf{a}_m^l\frac{\Gamma(2\nu+k+m)k!}{\Gamma(2\nu+k)(k-m)!}C_k^\nu(1). \tag{2.4}$$

Here, we have used $C_k^\nu(1) = \Gamma(k+2\nu)/[\Gamma(2\nu)k!]$ and have set

$$\mathsf{a}_m^l = \frac{2^m\Gamma(\nu+m)\Gamma(2\nu)}{\Gamma(\nu)\Gamma(2\nu+2m)}\mathsf{B}_{2l,m}(\zeta). \tag{2.5}$$

Now, it is a straightforward matter to show, using induction, that the recursively defined scalars b_j^m satisfy

$$\prod_{p=0}^{m-1}(X-p(p+2\nu)) = \sum_{j=1}^{m}\mathsf{b}_j^mX^j. \tag{2.6}$$

As a result, we can write the multiplicity functions as

$$\frac{\Gamma(2\nu+k+m)k!}{\Gamma(2\nu+k)(k-m)!} = \prod_{p=0}^{m-1}(k+2\nu+p)\prod_{p=0}^{m-1}(k-p) = \sum_{j=1}^{m}\mathsf{b}_j^m[k(k+2\nu)]^j. \tag{2.7}$$

Therefore, by combining (2.4) and (2.7), we arrive at the differential-spectral identity

$$\frac{d^{2l}}{d\theta^{2l}}\mathscr{C}_k^\nu(\cos\theta)\big|_{\theta=0} = \sum_{m=1}^{l}\mathsf{a}_m^l\sum_{j=1}^{m}\mathsf{b}_j^m[k(k+2\nu)]^j = \mathscr{P}_l^\nu(\lambda_k^\nu). \tag{2.8}$$

Applying the differential operator $\mathsf{P}(d/d\theta)$ by taking into account only its even order terms, combined with the above, at once gives the desired conclusion. $\square$

A straightforward set of calculations yield the first few polynomials $\mathscr{P}_l^\nu$, listed below for the convenience of the reader. Indeed, for $1 \leq l \leq 3$, we have

$$\mathscr{P}_1^\nu(X) = \frac{-X}{(2\,\nu+1)}, \quad \mathscr{P}_2^\nu(X) = \frac{3X^2 - 4\nu X}{4\,\nu^2 + 8\,\nu + 3}, \tag{2.9}$$

$$\mathscr{P}_3^\nu(X) = \frac{-15X^3 + 60\nu X^2 - 16(4\nu^2 + \nu)X}{8\,\nu^3 + 36\,\nu^2 + 46\,\nu + 15}, \tag{2.10}$$

while $\mathscr{P}_4^\nu(X)$ is given by

$$\frac{105X^4 - 840\nu X^3 + 336(7\nu^2 + 2\nu)X^2 - 64(34\nu^3 + 24\nu^2 + 5\nu)X}{16\nu^4 + 128\nu^3 + 344\nu^2 + 352\nu + 105}. \tag{2.11}$$

3. A trace formulation of the Maclaurin spectral coefficients. Being motivated to understand and describe the Macluarin spectral coefficients more explicitly and, in particular, to formulate and exploit their relationship to the well-known heat trace and the Minakshisundaram-Plejel heat coefficients, we now specialize to functions $\Phi = \Phi(X)$ of the Laplace transform type

$$\Phi(X) = \int_0^\infty e^{-Xs} f(s)\, ds, \quad X \geq 0, \tag{3.1}$$

for a suitable L^1-integrable function f. For Φ, as above, using Fubini's theorem to commute the integral and the summation, we can write the Maclaurin spectral coefficients b_{2l}^n in (1.7), by noting $\nu = (n-1)/2$, as

$$\begin{aligned} b_{2l}^n[\Phi] &= \int_0^\infty \sum_{k=0}^\infty M_k^n \sum_{j=1}^l \mathsf{c}_j^l [\lambda_k^n]^j e^{-\lambda_k^n s} f(s)\, ds \\ &= \int_0^\infty \sum_{j=1}^l \mathsf{c}_j^l (-1)^j f(s) \frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta} ds \\ &= \int_0^\infty f(s) \left[\mathscr{P}_l^\nu\left(-\frac{d}{ds}\right)\right] \operatorname{tr} e^{s\Delta} ds. \end{aligned} \tag{3.2}$$

As a result, we can now write the Macluarin spectral coefficients in the alternative and more suggestive trace form

$$b_{2l}^n = \operatorname{tr}[F_l^\nu(-\Delta)], \tag{3.3}$$

where F_l^ν is the function

$$F_l^\nu(X) := \int_0^\infty f(s)\mathscr{P}_l^\nu\Big(-\frac{d}{ds}\Big)e^{-sX}\,ds, \quad X \geq 0. \tag{3.4}$$

Theorem 3.1. *Let $n \geq 2$, and let $\Phi = \Phi(X)$ be as defined by the Laplace integral* (3.1) *for a suitable integrable f. Consider the Schwartzian kernel of $\Phi(-\Delta)$ and its expansion*

$$K_\Phi(\theta) = \frac{1}{\omega_n}\sum_{k=0}^\infty M_k^n \Phi(\lambda_k^n)\mathscr{C}_k^{(n-1)/2}(\cos\theta) = \frac{1}{\omega_n}\sum_{l=0}^\infty \frac{b_{2l}^n}{(2l)!}\theta^{2l}. \tag{3.5}$$

Then, the Maclaurin spectral coefficients $b_{2l}^n = b_l^n[\Phi]$ can be described by (3.2) *or, equivalently, by the trace formulation* (3.3)*–*(3.4)*.*

Now that we have bridged between the Maclaurin spectral coefficients $b_{2l}^n[\Phi]$ of the Schwartzian kernel K_Φ on one hand and an integral involving the heat trace $\operatorname{tr} e^{s\Delta}$ (cf., (3.2)–(3.3)) on the other, we go on to exploit this further by showing that the coefficients $b_{2l}^n[\Phi]$ can be described in terms of the classical Jacobi theta functions ϑ_1, ϑ_2. For the sake of the reader's convenience, we recall that these are defined for $s > 0$, respectively, by the theta series (cf., e.g., **[9, 27]**)

$$\vartheta_1(s) = 1 + \sum_{j=1}^\infty 2e^{-j^2 s} = \sqrt{\pi/s}\Big(1 + \sum_{j=1}^\infty 2e^{-j^2\pi^2/s}\Big), \tag{3.6}$$

(where the second equality results from an application of the Poisson summation formula) with asymptotics $\vartheta_1(s) = \sqrt{\pi/s} + O(e^{-1/s})$ as $s \searrow 0$, and

$$\vartheta_2(s) = \sum_{j=0}^\infty (2j+1)e^{-(j+(1/2))^2 s} \tag{3.7}$$

with asymptotics

$$\vartheta_2(s) \sim 1/s + \sum_{k=0}^\infty \mathtt{B}_k s^k/k!$$

as $s \searrow 0$ with $\mathtt{B}_k$ as in (4.12). We will see below that, in odd dimensions, it is the function ϑ_1 that will naturally arise and, in even dimensions, the function ϑ_2.

Theorem 3.2 ($n \geq 3$ odd)**.** *Let $\Phi = \Phi(X)$ be as in* (3.1)*. Then, for $n \geq 3$ odd, the Maclaurin spectral coefficients $b^n_{2l} = b^n_{2l}[\Phi]$ in* (3.2)–(3.3) *can be expressed by*

$$(3.8)\quad b^n_0 = \operatorname{tr}\Phi(-\Delta) = \sum_{m=0}^{(n-3)/2} \frac{\mathsf{A}^n_m (-1)^{m+1}}{(n-1)!} \int_0^\infty f(s)\vartheta_1^{(m+1)}(s)\, d\mu(s),$$

where $d\mu(s) = e^{s(n-1)^2/4} ds$ and, for $l \geq 1$, by

$$(3.9)\qquad \begin{aligned} b^n_{2l} &= \int_0^\infty f(s) \left[\mathscr{P}^\nu_l\left(-\frac{d}{ds}\right)\right] \operatorname{tr} e^{s\Delta} ds \\ &= \sum_{m=0}^{(n-3)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}^n_m \mathsf{c}^l_j (-1)^{j+m+1}}{(n-1)!} \binom{j}{i} [(n-1)/2)]^{2i} \\ &\quad\times \int_0^\infty f(s)\vartheta_1^{(m+j-i+1)}(s)\, d\mu(s). \end{aligned}$$

Here, c^l_j are as in Theorem 2.1*, A^n_m are scalars* (*see below*) *and $\vartheta_1^{(k)}$ is the kth derivative of the function ϑ_1 as defined by* (3.6)*.*

Proof. We proceed by first writing the heat trace $\Theta(s) = \operatorname{tr} e^{s\Delta}$ in terms of the Jacobi theta function. Towards this end, it will be convenient to express the multiplicity function M^k_n in the polynomial form

(3.10)

$$M^n_k = (n+2k-1)\frac{(k+n-2)!}{(n-1)!k!} = \sum_{m=0}^{(n-3)/2} \frac{2\mathsf{A}^n_m}{(n-1)!}(k+(n-1)/2)^{2m+2},$$

where the scalars A^n_m are taken as the coefficients of the polynomial identity

$$\prod_j (X^2 - j^2) = \sum_m \mathsf{A}^n_m X^{2m+2} \quad (0 \leq j,\ m \leq (n-3)/2).$$

Using the observation that the sum on the right here vanishes if X is an integer between 1 and $(n-3)/2$, we can write the heat trace as

$$(3.11)\qquad \Theta(s) = \operatorname{tr} e^{s\Delta} = \sum_{k=0}^{\infty} M^n_k e^{-k(k+n-1)s}$$

$$= \sum_{m=0}^{(n-3)/2} \frac{2\mathsf{A}_m^n}{(n-1)!} \sum_{p=1}^{\infty} p^{2m+2} e^{-s(p^2-(n-1)^2/4)}$$
$$= \sum_{m=0}^{(n-3)/2} \frac{(-1)^{m+1}\mathsf{A}_m^n}{(n-1)!} \vartheta_1^{(m+1)}(s) e^{s(n-1)^2/4}.$$

The proof of (3.8) and (3.9) can be completed by differentiating (3.11) using the Leibniz rule and plugging this into (3.2). □

Theorem 3.3 ($n \geq 2$ even)**.** *Let $\Phi = \Phi(X)$ be as in* (3.1)*. Then, for $n \geq 2$ even, the Maclaurin spectral coefficients $b_{2l}^n = b_{2l}^n[\Phi]$ in* (3.2)*–*(3.3) *can be expressed by*

$$b_0^n = \operatorname{tr} \Phi(-\Delta) = \sum_{m=0}^{(n-2)/2} \frac{\mathsf{B}_m^n (-1)^m}{(n-1)!} \int_0^\infty f(s) \vartheta_2^{(m)}(s)\, d\mu(s), \tag{3.12}$$

where $d\mu(s) = e^{s(n-1)^2/4} ds$ and, for $l \geq 1$, by

$$\begin{aligned} b_{2l}^n &= \int_0^\infty f(s) \left[\mathscr{P}_l^\nu \left(-\frac{d}{ds} \right) \right] \operatorname{tr} e^{s\Delta} ds \\ &= \sum_{m=0}^{(n-2)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}_m^n \mathsf{c}_j^l (-1)^{j+m}}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i} \\ &\quad \times \int_0^\infty f(s) \vartheta_2^{(m+j-i)}(s)\, d\mu(s). \end{aligned} \tag{3.13}$$

Here, c_j^l are as in Theorem 2.1*, B_m^n are scalars* (*see below*) *and $\vartheta_2^{(k)}$ is the kth derivative of the function ϑ_2 as defined by* (3.7)*.*

Proof. The proof of (3.12) and (3.13) when n is even is very similar to those in the previous theorem, and thus, below, we focus on the main differences only. Indeed, here, we proceed by writing the multiplicity function M_n^k as a polynomial

$$M_k^n = \frac{2k+n-1}{(n-1)!} \prod_{j=1}^{n-2} (k+j) = \frac{(2k+n-1)}{(n-1)!} \sum_{m=0}^{(n-2)/2} \mathsf{B}_m^n (k+(n-1)/2)^{2m}, \tag{3.14}$$

where the scalars B_m^n are taken as coefficients of the polynomial identity

$$\prod_j [X^2 - (j-1/2)^2] = \sum_m \mathsf{B}_m^n X^{2m}$$

(with $1 \leq j \leq (n-2)/2$, $0 \leq m \leq (n-2)/2$) when $n \geq 4$, whilst, for $n = 2$, the identity on the second line holds trivially with $\mathsf{B}_0^2 = 1$. Using the observation that the sum on the right here vanishes if X is an integer between 1 and $(n-2)/2$, we can write the heat trace as

$$\begin{aligned} \Theta(s) = \operatorname{tr} e^{s\Delta} &= \sum_{k=0}^{\infty} M_k^n e^{-k(k+n-1)s} \\ &= \sum_{m=0}^{(n-2)/2} \frac{2\mathsf{B}_m^n}{(n-1)!} \sum_{p=1/2}^{\infty} p^{2m+1} e^{-s(p^2-(n-1)^2/4)} \\ &= \sum_{m=0}^{(n-2)/2} \frac{(-1)^m \mathsf{B}_m^n}{(n-1)!} \vartheta_2^{(m)}(s) e^{s(n-1)^2/4}. \end{aligned} \tag{3.15}$$

The remainder of the argument is similar to that given in Theorem 3.2, and hence, is abbreviated. $\square$

For the sake of future reference, note that, in the case of the heat kernel (with $\Phi_s(X) = e^{-sX}$) proceeding directly from (3.11)–(3.15) and using the relation $b_{2l}^n[\Phi_s] = b_{2l}^n(s) = \mathscr{P}_l^\nu(-d/ds) \operatorname{tr} e^{s\Delta}$, we have, for $l \geq 1$:

- for $n \geq 3$ odd, b_{2l}^n is given by

(3.16)
$$\sum_{m=0}^{(n-3)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}_m^n \mathsf{c}_j^l (-1)^{m+j+1}}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i} \vartheta_1^{(m+j-i+1)} e^{s(n-1)^2/4};$$

- for $n \geq 2$ even, b_{2l}^n is given by

(3.17)
$$\sum_{m=0}^{(n-2)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}_m^n \mathsf{c}_j^l (-1)^{m+j}}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i} \vartheta_2^{(m+j-i)} e^{s(n-1)^2/4}.$$

Naturally, here, we have $b_0^n(s) = \Theta(s) = \operatorname{tr} e^{s\Delta}$ as in (3.11) and (3.15), respectively.

4. Asymptotic analysis of Schwartzian kernels via Jacobi functions. Following from the discussion and representation results in the previous section, here, we consider a one-parameter family of functions $\Phi_\sigma = \Phi_\sigma(X)$ (with $\sigma > 0$, $X \geq 0$) defined through a Laplace type integral

$$\Phi_\sigma(X) = \int_0^\infty e^{-Xs} f_\sigma(s)\, ds, \quad X \geq 0, \tag{4.1}$$

where $f_\sigma = fe^{-\sigma s}$ while $|f| \leq c(1+s^a)$ for some $c > 0$, $a \geq 1$ and all $s > 0$. We aim to describe the asymptotics of $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ as $\sigma \nearrow \infty$ by connecting firstly to the short time behavior of the heat trace $\Theta(t) = \operatorname{tr} e^{t\Delta}$ and invoking the Minakshisundaram-Pleijel heat coefficients and secondly to the previously encountered Jacobi theta series and their short time asymptotics, respectively.

Theorem 4.1. *The Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$, with Φ_σ as in* (4.1)*, satisfy the asymptotics as $\sigma \nearrow \infty$*

$$b^n_0(\sigma) = \operatorname{tr} \Phi_\sigma(-\Delta) \sim \sum_{k=0}^\infty \frac{a^n_k}{(4\pi)^{n/2}} \int_0^\infty f(s) s^{k-n/2} e^{-\sigma s} ds, \tag{4.2}$$

and, for $l \geq 1$ with $\nu = (n-1)/2$,

(4.3)

$$\begin{aligned} b^n_{2l}(\sigma) &= \operatorname{tr}[\Phi_\sigma \mathscr{P}^\nu_l](-\Delta) \\ &\sim \sum_{j=1}^{l} \sum_{k=0}^\infty \frac{(-1)^j \mathsf{c}^l_j(\nu)\Gamma(k-n/2+1) a^n_k}{(4\pi)^{n/2}\Gamma(k-n/2-j+1)} \int_0^\infty f(s) s^{k-j-n/2} e^{-\sigma s} ds. \end{aligned}$$

Proof. Starting from the short time asymptotics of the heat trace (1.2), see **[24]** for $s > 0$, we have

$$\begin{aligned} \Theta(s) = \operatorname{tr} e^{s\Delta} &= \sum_{k=0}^\infty (2k+n-1) \frac{(k+n-2)!}{k!(n-1)!} e^{-sk(k+n-1)} \\ &= \sum_{k=0}^\infty \frac{a^n_k s^k}{(4\pi s)^{n/2}} + O(e^{-1/s}). \end{aligned} \tag{4.4}$$

Therefore, successive differentiation with respect to the s-variable results in the expression

$$\left(-\frac{d}{ds}\right)^j \operatorname{tr} e^{s\Delta} = \sum_{k=0}^{\infty} \frac{(-1)^j \Gamma(k-n/2+1) a_k^n}{(4\pi)^{n/2}\Gamma(k-n/2-j+1)} s^{k-j-n/2} + O(e^{-1/s}).$$

Now, referring to the trace formulation of the Maclaurin spectral coefficients $b_{2l}^n(\sigma) = b_{2l}^n[\Phi_\sigma]$ as in (3.2), we obtain, upon using this last heat trace derivative identity, the description and asymptotics as $\sigma \nearrow \infty$

(4.5)

$$\begin{aligned} b_{2l}^n(\sigma) &= \int_0^\infty f_\sigma(s) \left[\mathscr{P}_l^\nu\left(-\frac{d}{ds}\right)\right] \operatorname{tr} e^{s\Delta} ds \\ &= \int_0^\infty f_\sigma(s) \sum_{j=1}^{l} \mathsf{c}_j^l(\nu) \left(-\frac{d}{ds}\right)^j \operatorname{tr} e^{s\Delta} ds \\ &\sim \sum_{j=1}^{l} \frac{(-1)^j \mathsf{c}_j^l(\nu)}{(4\pi)^{n/2}} \sum_{k=0}^{\infty} \frac{\Gamma(k-n/2+1) a_k^n}{\Gamma(k-j-n/2+1)} \int_0^\infty f(s) s^{k-j-n/2} e^{-\sigma s} ds. \end{aligned}$$

Indeed, to justify the last line, we proceed as follows. First, by using the bound on the derivatives of the heat trace $|d^j\Theta(s)/ds^j| \le cs^{-j-n/2}$ (see Appendix C for a proof of this bound) we write, for fixed $t > 0$,

$$\left| \left\{ \int_0^\infty - \int_0^t \right\} f_\sigma(s) \frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta} ds \right| \le \int_t^\infty |f(s)| s^{-j-n/2} e^{-\sigma s} ds.$$

Next, bounding the integral on the right using the bound on f, we can write

(4.6)

$$\begin{aligned} \int_t^\infty |f(s)| s^{-j-n/2} e^{-\sigma s} ds &\le ce^{-bt} \int_t^\infty s^{a-j-n/2} e^{-s(\sigma-b)}\, ds \\ &\le \frac{ce^{-bt}}{(\sigma-b)^{a-j-n/2+1}} \int_{(\sigma-b)t}^\infty u^{a-j-n/2} e^{-u} du \end{aligned}$$

where, upon taking $b = \sqrt{|\sigma|}$, $t = 1$, it is seen that this is of order $O(e^{-\sqrt{|\sigma|}})$. Substituting for $e^{s\Delta}$ and its derivatives in $(0,t)$, using (1.2) and then bounding the remaining integral in an analogous manner, gives the desired conclusion. □

Theorem 4.2. *Let $n \geq 3$ be odd, and let Φ_σ be defined by* (4.1) *with f_σ as above. Then, the Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ satisfy, as $\sigma \nearrow \infty$:*

(4.7)
$$b^n_0(\sigma) = \operatorname{tr}\Phi_\sigma(-\Delta) \sim \sum_{m=0}^{(n-3)/2} \frac{\mathsf{A}^n_m \Gamma(m+3/2)}{(n-1)!} \int_0^\infty f(s) s^{-m-3/2} e^{-\sigma s} d\mu,$$

where $d\mu(s) = e^{s(n-1)^2/4} ds$ and, for $l \geq 1$,

(4.8)
$$b^n_{2l}(\sigma) = \operatorname{tr}[\Phi_\sigma \mathscr{P}^\nu_l](-\Delta) \sim \sum_{m=0}^{(n-3)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}^n_m \mathsf{c}^l_j (-1)^i}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i}$$
$$\times \Gamma(m+j-i+3/2) \int_0^\infty f(s) s^{-m-j+i-3/2} e^{-\sigma s} d\mu,$$

where A^n_m are the scalars as defined Theorem 3.2.

Proof. Referring to (3.6), we have the asymptotics $\vartheta_1(s) = \sqrt{\pi/s} + O(e^{-1/s})$ as $s \searrow 0$. As a result, by successive differentiation for $m \geq 0$, we have, for $s \searrow 0$

$$\begin{aligned} \vartheta_1^{(m+1)}(s) &= (-1)^{m+1} \frac{(2m+1)!!}{2^{m+1}} \sqrt{\pi} s^{-m-3/2} + O(e^{-1/s}) \\ &= (-1)^{m+1} \Gamma(m+3/2) s^{-m-3/2} + O(e^{-1/s}). \end{aligned} \tag{4.9}$$

Upon substituting these into (3.9) and using the assumptions on f_σ, the required asymptotics follow by invoking the same argument as in Theorem 4.1. □

Theorem 4.3. *Let $n \geq 2$ be even, and let Φ_σ be defined by* (4.1) *with f_σ as above. Then, the Maclaurin spectral coefficients $b^n_{2l}(\sigma) = b^n_{2l}[\Phi_\sigma]$ satisfy, as $\sigma \nearrow \infty$*

$$b^n_0(\sigma) = \operatorname{tr}\Phi_\sigma(-\Delta) \sim \sum_{m=0}^{(n-2)/2} \frac{\mathsf{B}^n_m}{(n-1)!} \tag{4.10}$$

$$\times \int_0^\infty f(s)\left[\frac{m!}{s^{1+m}} + \sum_{k=m}^{\infty} \frac{(-1)^m \mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)}\right] e^{-\sigma s} d\mu,$$

where $d\mu(s) = e^{s(n-1)^2/4} ds$, *and, for* $l \geq 1$,

(4.11)

$$b_{2l}^n(\sigma) = \operatorname{tr}[\Phi_\sigma \mathscr{P}_l^\nu](-\Delta) \sim \sum_{m=0}^{(n-2)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{B}_m^n \mathsf{c}_j^l (-1)^{j+m}}{(n-1)!} \binom{j}{i} [(n-1)/2]^{2i}$$
$$\times \left\{ \int_0^\infty f(s) \frac{(-1)^{(m+j-i)}(m+j-i)!}{s^{m+j-i+1} e^{\sigma s}} d\mu \right.$$
$$\left. + \int_0^\infty f(s) \sum_{k=(m+j-i)}^{\infty} \frac{\mathsf{B}_k s^{k-m-j+i} e^{-\sigma s}}{\Gamma(k-m-j+i+1)} d\mu \right\},$$

where B_k *are the Bernoulli numbers as defined by* (4.12), *and* B_m^n *are the scalars defined in Theorem* 3.3.

Proof. It is sufficient here to use the fact that the theta series defining ϑ_2 satisfies the asymptotics as $s \searrow 0$

$$\vartheta_2(s) \sim \frac{1}{s} + \sum_{k=0}^{\infty} \frac{\mathsf{B}_k s^k}{k!}, \tag{4.12}$$

$$\mathsf{B}_k = \frac{(-1)^k}{(k+1)} B_{2k+2}(1 - 2^{-2k-1}),$$

where B_m are the well-known Bernoulli numbers, and likewise, by further differentiating that

$$\vartheta_2^{(m)}(s) \sim \frac{(-1)^m m!}{s^{1+m}} + \sum_{k=m}^{\infty} \frac{\mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)} \tag{4.13}$$

as $s \searrow 0$ (cf., **[9, 27]**). Substituting these into (3.13) and using the assumptions on f_σ leads to (4.11). □

4.1. Trace asymptotics and resolvent powers. As an application, here we discuss the asymptotics of powers of the resolvent corresponding to taking $f_\sigma(s) = s^{a-1} e^{-s\sigma}/\Gamma(a)$ for $a > 1$. Through a limiting process, these will then be used to obtain the asymptotics for the Maclaurin spectral coefficients of the heat kernel, that is, $b_{2l}^n[\Phi = e^{-tX}]$. Indeed, let

$$\Phi_\sigma(X) = \int_0^\infty \frac{s^{a-1}e^{-s\sigma}}{\Gamma(a)} e^{-sX}\,ds = (\sigma + X)^{-a}. \tag{4.14}$$

Then, $\Phi_\sigma(-\Delta) := R_\sigma^a$ is the resolvent operator to the power a. By applying the theorems of Section 4, we can obtain the asymptotics of the Maclaurin spectral coefficients $b_{2l}^n(\sigma, a) = b_{2l}^n[R_\sigma^a]$ as $\sigma \nearrow \infty$. Towards this end, note that Theorem 4.1 gives (for $l \geq 1$)

(4.15)

$$b_{2l}^n(\sigma, a) \sim \sum_{j=0}^{l} \sum_{k=0}^{\infty} \frac{(-1)^j \mathsf{c}_j^l(\nu)\Gamma(k - n/2 + 1)\Gamma(a + k - j - n/2)}{(4\pi)^{n/2}\Gamma(k - n/2 - j + 1)\Gamma(a)\sigma^{a+k-j-n/2}}\, a_k^n.$$

Alternatively, by invoking the theta function description of the Maclaurin spectral coefficients, we have the following asymptotics by considering the cases of odd and even n separately.

- For $n \geq 3$ odd, Theorem 4.2 yields:

(4.16)

$$b_0^n(\sigma, a) \sim \sum_{m=0}^{(n-3)/2} \frac{\mathsf{A}_m^n \Gamma(m + 3/2)}{(n-1)!\Gamma(a)}\, \Gamma(a - m - 3/2)(\sigma - (n-1)^2/4)^{m-a+3/2},$$

and, for $l \geq 1$,

(4.17)

$$\begin{aligned} b_{2l}^n(\sigma, a) \sim &\sum_{m=0}^{(n-3)/2} \sum_{j=1}^{l} \sum_{i=0}^{j} \frac{\mathsf{A}_m^n \mathsf{c}_j^l (-1)^i}{(n-1)!\Gamma(a)} \binom{j}{i} [(n-1)/2]^{2i} \Gamma(m + j - i + 3/2) \\ &\times \Gamma(a + i - m - j - 3/2)(\sigma - (n-1)^2/4)^{m+j-i-a+3/2}. \end{aligned}$$

- For $n \geq 2$ even, Theorem 4.3 yields

(4.18)

$$\begin{aligned} b_0^n(\sigma, a) \sim &\sum_{m=0}^{(n-2)/2} \frac{\mathsf{B}_m^n}{(n-1)!\Gamma(a)} \\ &\times \Bigg\{ m!\Gamma(a - 1 - m)(\sigma - (n-1)^2/4)^{1-a+m} \\ &\qquad + \sum_{k=m}^{\infty} (-1)^m \frac{\mathsf{B}_k \Gamma(a + k - m)}{\Gamma(k - m + 1)} (\sigma - (n-1)^2/4)^{-a-k+m} \Bigg\}, \end{aligned}$$

and, for $l \geq 1$,

(4.19)

$$
\begin{aligned}
&b^n_{2l}(\sigma,a)\\
&\quad\sim \sum_{m=0}^{(n-2)/2}\sum_{j=1}^{l}\sum_{i=0}^{j}\frac{\mathsf{B}^n_m\mathsf{c}^l_j(-1)^{j+m}}{(n-1)!\Gamma(a)}\binom{j}{i}[(n-1)/2]^{2i}\\
&\quad\times\bigg\{(-1)^{(m+j-i)}(m+j-i)!\Gamma(a-1-m-j+i)(\sigma-(n-1)^2/4)^{1-a+m+j-i}\\
&\qquad+\sum_{k=(m+j-i)}^{\infty}\frac{\mathsf{B}_k\Gamma(a+k-m-j+i)}{\Gamma(k-m-j+i+1)}(\sigma-(n-1)^2/4)^{-a-k+m+j-i}\bigg\}.
\end{aligned}
$$

The asymptotics of $b^n_0(\sigma,a)$ as $\sigma\nearrow\infty$ now give the short time asymptotics of the heat trace. Indeed, this follows by first noting $\Theta(s)=\operatorname{tr}e^{s\Delta}=\lim(k/s)^k\operatorname{tr}R^k_{k/s}=\lim(k/s)^k b^n_0(k/s,k)$ as $k\nearrow\infty$ for $s>0$ and then recalling $e^{-x}=\lim(1+x/k)^{-k}$ and $\lim\Gamma(k+\alpha)/[\Gamma(k)k^\alpha]=1$ as $k\nearrow\infty$ for $\alpha\in\mathbb{R}$. Now, for $n\geq 3$ odd using (4.16), this leads to (as $s\searrow 0$)

$$
\operatorname{tr}e^{s\Delta}\sim e^{s(n-1)^2/4}\sum_{m=0}^{(n-3)/2}\frac{\mathsf{A}^n_m\Gamma(m+3/2)}{(n-1)!}s^{-m-3/2}, \tag{4.20}
$$

and, in a similar fashion for $n\geq 2$ even using (4.19), this leads to (as $s\searrow 0$)

$$
\begin{aligned}
\operatorname{tr}e^{s\Delta}\sim e^{s(n-1)^2/4}+&\sum_{m=0}^{(n-2)/2}\frac{\mathsf{B}^n_m(-1)^m}{(n-1)!}\\
&\times\bigg\{(-1)^m(m!)s^{-m-1}+\sum_{k=m}^{\infty}\frac{\mathsf{B}_k s^{k-m}}{\Gamma(k-m+1)}\bigg\}.
\end{aligned} \tag{4.21}
$$

Compare with (3.11)–(3.15) and (3.16)–(3.17).

5. Dirichlet energy and extension by semigroups. In this section, we apply some of the tools developed earlier to build and study extension operators out of semigroups $(T_t : t>0)$ generated by functions of the spherical Laplacian and some energy inequalities resulting from them. Here, the extension operator extends functions on the n-sphere $\mathbb{S}$, seen as the boundary of the open unit ball $\mathbb{B}=$

$\{(x_1, \ldots, x_{n+1}) : |x| < 1\}$ to functions inside the ball by a fixed semigroup, and the aim is to examine the associated energy inequalities by invoking the Maclaurin spectral coefficients and the classical Funk-Hecke identity. For the sake of this exposition, we confine to the Dirichlet energy and the Dirichlet principle, asserting that, for all $f \in H^{1/2}(\mathbb{S}) \subset L^2(\mathbb{S})$ and with u_H denoting the harmonic extension of f to $\mathbb{B}$, we have

$$\int_{\mathbb{B}} |\nabla u|^2 \geq \int_{\mathbb{B}} |\nabla u_H|^2 \quad \text{for all } u \in H^1(\mathbb{B}) : u|_{\partial \mathbb{B}} = f. \tag{5.1}$$

Towards this end, let $F = F(X)$ be a non-negative function in the Borel functional calculus of the spherical Laplacian Δ, and, for $0 < r \leq 1$, consider the associated one-parameter family of functions $\Phi_r = \Phi_r(X)$, defined as

$$\Phi_r(X) = r^{F(X)}. \tag{5.2}$$

The operator family $(\Phi_r(-\Delta) : 0 < r \leq 1)$ is then a semigroup in $L^2(\mathbb{S})$; in fact, the substitution $r = e^{-t}$ shows that $\Phi_r(-\Delta)$ is a re-parametrization of the semigroup $(T_t = e^{-tF(-\Delta)} : t \geq 0)$. Now, writing the expansion of f in spherical harmonics $f = \sum_{k=0}^{\infty} Y_k$, where Y_k are the spherical harmonics of degree k, we define the extension u_F of f to be

$$\begin{aligned} u_F(rx) = \Phi_r(-\Delta) f(x) &= \sum_{k=0}^{\infty} r^{F(\lambda_k^n)} Y_k(x) \\ &= \int_{\mathbb{S}} K_{\Phi_r}(x, y) f(y) \, d\mathcal{H}^n(y), \quad x \in \mathbb{S}, \ 0 < r \leq 1, \end{aligned} \tag{5.3}$$

where K_{Φ_r} is the Schwartzian kernel of $\Phi_r(-\Delta)$ (cf., (5.9) for a formulation). Note that, upon taking $F = H$ with H, the function

$$H(X) := \left(X + \left(\frac{n-1}{2} \right)^2 \right)^{1/2} - \frac{n-1}{2}, \quad X \geq 0, \tag{5.4}$$

we have $H(\lambda_k^n) = k$ for all $k \geq 0$, and subsequently, u_H is precisely the harmonic extension of f to the unit ball. Now, using the identity

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \int_0^1 \int_{\mathbb{S}} \left[|\partial_r u_F|^2 - \frac{1}{r^2} u_F \Delta_{\mathbb{S}} u_F \right] r^n d\mathcal{H}^n dr, \tag{5.5}$$

it can be seen that the Dirichlet energy of u_F as defined by (5.3) can be expressed as

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \left[\frac{F(\lambda_k^n)^2 + \lambda_k^n}{2F(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n. \tag{5.6}$$

In particular, the energy of the harmonic extension u_H can be seen to be

$$\begin{aligned} \int_{\mathbb{B}} |\nabla u_H|^2 &= \sum_{k=0}^{\infty} \left[\frac{H(\lambda_k^n)^2 + \lambda_k^n}{2H(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n \\ &= \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n = \|f\|^2_{H^{1/2}(\mathbb{S})}. \end{aligned} \tag{5.7}$$

Thus, in view of $u_F = u_H = f$, on $\partial\mathbb{B}$, the Dirichlet principle is a formulation of the inequality

$$\sum_{k=0}^{\infty} \left[\frac{F(\lambda_k^n)^2 + \lambda_k^n}{2F(\lambda_k^n) + n - 1} \right] \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n. \tag{5.8}$$

Now, we make use of the Funk-Hecke identity to give an alternative description of the Dirichlet energy of u_F by invoking the Maclaurin spectral coefficients. Towards this end, the Schwartzian kernel of $\Phi_r(-\Delta)$ may be written via Gegenbauer polynomials as

(5.9)

$$\begin{aligned} K_{\Phi_r}(x,y) &= \frac{1}{\omega_n} \sum_{k=0}^{\infty} M_k^n \Phi_r(\lambda_k^n) \mathscr{C}_k^{(n-1)/2}(\cos\theta) \\ &= \frac{1}{\omega_n} \sum_{k=0}^{\infty} (2k+n-1) \frac{(k+n-2)!}{k!(n-1)!} r^{F(\lambda_k^n)} \mathscr{C}_k^{(n-1)/2}(\cos\theta), \end{aligned}$$

where, as before, $\theta = \cos^{-1}(x \cdot y)$ is the geodesic distance between x and y. By formally writing the Maclaurin expansion of the kernel K_{Φ_r}, we have

(5.10)

$$\sum_{k=0}^{\infty} (2k+n-1) \frac{(k+n-2)!}{k!(n-1)!} r^{F(\lambda_k^n)} \mathscr{C}_k^{(n-1)/2}(\cos\theta) = \sum_{l=0}^{\infty} \frac{b_{2l}^n(r)}{(2l)!} \theta^{2l},$$

where the Maclaurin spectral coefficients $b^n_{2l}(r) = b^n_{2l}[\Phi_r]$, by referring to the earlier trace formulation, can be described as

$$b^n_{2l}(r) = \sum_{k=0}^{\infty} M^n_k \Phi_r(\lambda^n_k) \sum_{j=1}^{l} \mathsf{c}^l_j [\lambda^n_k]^j = \sum_{k=0}^{\infty} M^n_k [\Phi_r \mathscr{P}_l](\lambda^n_k). \tag{5.11}$$

Using the Funk-Hecke formula on the integral operator below (cf., **[18]** or **[19, 22]**), we have:

$$\begin{aligned} u_F(rx) &= \int_{\mathbb{S}^n} K_{\Phi_r}(x,y) f(y)\, d\mathcal{H}^n(y) \\ &= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty} \frac{b^n_{2l}(r)}{\omega_n (2l)!} \int_{\mathbb{S}^n} [\cos^{-1}(x\cdot y)]^{2l} Y_k(y)\, d\mathcal{H}^n(y) \\ &= \sum_{l=0}^{\infty}\sum_{k=0}^{\infty} \frac{\mu^l_k b^n_{2l}(r)}{\omega_n (2l)!} Y_k(x), \quad x \in \mathbb{S},\ r<1, \end{aligned} \tag{5.12}$$

where the coefficients μ^l_k are explicitly given by the weighted integral

$$\mu^l_k = \omega_{n-1} \int_{-1}^{1} [\cos^{-1} t]^{2l} \mathscr{C}^{(n-1)/2}_k(t)(1-t^2)^{(n-2)/2} dt, \quad l \ge 0. \tag{5.13}$$

Invoking (5.1) and (5.5) and directly comparing the expansions in spherical harmonics of the extension u_F given by (5.3) with (5.12) leads at once to the following statement.

Theorem 5.1. *Given $F = F(X)$ as above and $f \in H^{1/2}(\mathbb{S})$, let $u_F = r^{F(-\Delta)} f$ denote the extension of f as defined by* (5.3). *Then, the Dirichlet energy of u_F can be written as the weighted sum*:

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \int_0^1 \left[\gamma'^2_k(r) + \frac{1}{r^2}\gamma^2_k(r)\lambda^n_k\right] r^n dr \int_{\mathbb{S}} |Y_k|^2 d\mathcal{H}^n, \tag{5.14}$$

where the functions $\gamma_k = \gamma_k(r)$ and the Maclaurin spectral coefficients $b^n_{2l}(r) = b^n_{2l}[r^{F(-\Delta)}]$ satisfy the trace formulation

$$\gamma_k(r) = \sum_{l=0}^{\infty} \frac{b^n_{2l}(r)}{(2l)!} \mu^l_k = \operatorname{tr}\left[\sum_{l=0}^{\infty} \frac{\mu^l_k}{(2l!)} r^{F(-\Delta)} P_l(-\Delta)\right] = r^{F(\lambda^n_k)}, \tag{5.15}$$

with the sequence μ_k^l given by (5.13). *Furthermore, we have the energy inequality*

(5.16)
$$\sum_{k=0}^{\infty}\int_0^1\left[\gamma_k'^2(r)+\frac{1}{r^2}\gamma_k^2(r)\lambda_k^n\right]r^n dr\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n \geq \sum_{k=0}^{\infty}k\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n.$$

In particular, in view of the arbitrariness of the boundary function $f \in L^2(\mathbb{S})$, or else a direct variational argument, the above energy inequality results in the following.

Corollary 5.2. *Let $\gamma_k = \gamma_k(r)$ be as given by the trace formulation* (5.15), *and set $h_k(r) = r^k$. Then, for all $k \geq 0$, we have $\mathbb{E}_k[\gamma_k] \geq \mathbb{E}_k[h_k]$, that is,*

$$\int_0^1\left[\gamma_k'^2(r)+\frac{\lambda_k^n}{r^2}\gamma_k^2(r)\right]r^n dr \geq \int_0^1\left[h_k'^2(r)+\frac{\lambda_k^n}{r^2}h_k^2(r)\right]r^n dr. \tag{5.17}$$

Here, $\lambda_k^n = k(n+k-1)$ are the distinct eigenvalues of the spherical Laplacian, while, by direct verification, $\mathbb{E}_k[h_k] = k$.

Proof. Fix $k \geq 0$, and let g in $H^1(0,1)$ satisfy $g(0) = 0$, $g(1) = 1$. Then, firstly, for $h = h_k$, as above, it is seen that $-d/dr[r^n h_k'(r)] + \lambda_k^n r^{n-2} h_k(r) = 0$. Secondly, upon writing $g = h + \phi$ with $\phi \in H_0^1(0,1)$ and invoking the quadratic nature of the energy, we can write $\mathbb{E}_k[g] = \mathbb{E}_k[h+\phi] = \mathbb{E}_k[h] + \mathbb{E}_k[\phi] \geq \mathbb{E}_k[h] = k$ with the last inequality being *strict* for non-zero ϕ. Thus, $h = h_k$ is the unique minimizer of $\mathbb{E}_k$ with respect to its own boundary conditions. $\square$

Now, to finish off the section, we give a few examples to illustrate the above discussion of energy inequalities in some specific cases.

• If $F(X) \equiv s$ for some fixed $s \in [0,\infty)$, then u_F is the homogeneous degree s extension of f, that is, $u_F(rx) = r^s f(x)$ and

$$\begin{aligned}\int_{\mathbb{B}}|\nabla u_F|^2 &= \sum_{k=0}^{\infty}\frac{s^2+\lambda_k^n}{2s+n-1}\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n \\ &= \frac{s^2\|f\|_{L^2(\mathbb{S})}^2+\|\nabla f\|_{L^2(\mathbb{S})}^2}{2s+n-1} \geq \sum_{k=0}^{\infty}k\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n.\end{aligned} \tag{5.18}$$

Interestingly, taking the infimum on the left over $s \geq 0$ and rearranging terms leads to the inequality

$$\sqrt{(n-1)^2\|f\|^4_{L^2(\mathbb{S})} + 4\|\nabla f\|^2_{L^2(\mathbb{S})}\|f\|^2_{L^2(\mathbb{S})}} \geq \sum_{k=0}^{\infty}(2k+n-1)\int_{\mathbb{S}}|Y_k|^2.$$

• If $F(X) = X$, then $F(-\Delta)$ is the spherical Laplacian, and $u_F = e^{t\Delta}f$ with $t = \log 1/r$ is the heat extension of f. Here, $\gamma_k(r) = r^{k(k+n-1)}$, and

$$\int_{\mathbb{B}} |\nabla u_F|^2 = \sum_{k=0}^{\infty} \frac{\lambda_k^n(1+\lambda_k^n)}{2\lambda_k^n + n - 1}\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n. \tag{5.19}$$

• Choose $F_s(X)$ such that $F_s(\lambda_k^n) = sk$ for some fixed $s \in [0,\infty)$. (Note that $u_{F_1} = u_H$ is the harmonic extension of f.) Then, $\gamma_k(r) = r^{sk}$, and we have

$$\int_{\mathbb{B}} |\nabla u_{F_s}|^2 = \sum_{k=0}^{\infty} \frac{k(s^2k+k+n-1)}{2\,sk+n-1}\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n \geq \sum_{k=0}^{\infty} k\int_{\mathbb{S}}|Y_k|^2 d\mathcal{H}^n.$$

Remark 5.3. The last inequality is saturated, that is, it turns to an equality when $s = 1$.

APPENDIX

In this appendix, we gather together some of the results and calculations relating to the Gegenbauer and Bell polynomials that appeared earlier in the paper.[1]

A. Gegenbauer polynomials C_k^ν $(k \geq 0,\ \nu > -1/2)$. The Gegenbauer, or ultraspherical polynomial, $C_k^\nu(t)$ $(k \geq 0,\ \nu > -1/2)$ is defined by the coefficient of α^k in the generating function relation

$$\frac{1}{(1-2t\alpha+\alpha^2)^\nu} = \sum_{k=0}^{\infty} C_k^\nu(t)\alpha^k. \tag{A.1}$$

It has a truncated series representation resulting from the series solution to the Gegenbauer differential equation (see below) in the form

$$C_k^\nu(t) = \sum_{0\le l\le k/2} (-1)^l \frac{\Gamma(k-l+\nu)}{\Gamma(\nu)l!(k-2l)!}(2t)^{k-2l}, \tag{A.2}$$

and, most notably, the derivatives satisfy the recursive relation

$$\frac{d^m}{dt^m}C_k^\nu(t) = 2^m \frac{\Gamma(\nu+m)}{\Gamma(\nu)}\, C_{k-m}^{\nu+m}(t). \tag{A.3}$$

The polynomial $y = C_k^\nu(t)$ is a solution to the second-order homogenous differential equation (the Gegenbauer equation)

$$(1-t^2)\frac{d^2y}{dt^2} - (2\nu+1)t\frac{dy}{dt} + k(k+2\nu)\, y = 0, \tag{A.4}$$

that constitute a regular Sturm-Liouville system on the interval $(-1,1)$. The corresponding Gegenbauer operator is seen to be a positive self-adjoint second order differential operator in the weighted Lebesgue-Hilbert space $L^2(-1,1;(1-t^2)^{\nu-1/2}dt)$ having the discrete spectrum $\lambda_k = k(k+2\nu) : k \ge 0$ with associated eigenfunctions $y = C_k^\nu(t)$. In particular, upon setting $d\mu = (1-t^2)^{\nu-1/2}dt$, we have the orthogonality relations

$$\begin{aligned}(C_k^\nu, C_m^\nu)_{L^2(d\mu)} &= \int_{-1}^1 C_k^\nu(t)C_m^\nu(t)(1-t^2)^{\nu-1/2}dt \\ &= \frac{\pi 2^{1-2\nu}\Gamma(2\nu+m)}{m!(m+\nu)\Gamma(\nu)^2}\delta_{km}, \quad k,m\ge 0,\end{aligned} \tag{A.5}$$

where δ_{km} denotes the Kronecker delta. By direct evaluation, using (A.2) or otherwise, we have the pointwise identities $C_k^\nu(1) = (2\nu)_k/k!$ and $C_k^\nu(-t) = (-1)^k C_k^\nu(t)$, where $(x)_k = \Gamma(x+k)/\Gamma(x)$. When necessary, we use the normalized form of the polynomial defined by

$$\mathscr{C}_k^\nu(t) = \frac{C_k^\nu(t)}{C_k^\nu(1)}, \quad C_k^\nu(1) = \frac{\Gamma(2\nu+k)}{\Gamma(2\nu)k!}. \tag{A.6}$$

B. The Bell polynomial $\mathsf{B}_{m,j}$ and the vanishing of $\mathsf{B}_{2l,j}$ for $l \ge 1$, $j \ge l+1$. In order to describe the action of the differential operator $\mathscr{L} = \mathsf{P}(d/d\theta)$ associated with the polynomial $\mathsf{P} = \mathsf{P}_d(X)$ of degree $d \ge 2$ on the Gegenbauer polynomials, we will make use of Faà di Bruno's formula, a generalized chain rule, to write derivatives of $\mathscr{C}_k^\nu$

in terms of the (incomplete) Bell polynomials. Recall that, for a pair of positive integers m, j, the Bell polynomial $\mathsf{B}_{m,j}$ is the multi-variable polynomial defined for $x = (x_1, \dots, x_{m-j+1})$ as

$$\mathsf{B}_{m,j}(x) = \sum \frac{m!}{k_1!k_2!\cdots k_{m-j+1}!} \prod_{i=1}^{m-j+1} \left(\frac{x_i}{i!}\right)^{k_i}, \tag{B.1}$$

where the sum is taken over all sequences of non-negative integers $k_1, \dots, k_{m-j+1}$ such that[2]

$$k_1 + \cdots + j_{m-j+1} = j, \tag{B.2}$$

and

$$k_1 + 2k_2 + \cdots + (m-j+1)k_{m-j-1} = m.$$

For smooth functions f, g and $m \geq 1$, Faà di Bruno's formula then asserts that

$$\frac{d^m}{dx^m} f(g(x)) = \sum_{j=1}^{m} f^{(j)}(g(x)) \cdot \mathsf{B}_{m,j}(g'(x), g''(x), \dots, g^{(m-j+1)}(x)). \tag{B.3}$$

We now make the following, useful observation which will simplify certain applications of Faà di Bruno's formula.

Lemma B.1. $\mathsf{B}_{2l,j}(0, x_2, x_3, \dots, x_{2l-j+1}) \equiv 0$ *for* $l \geq 1$ *when* $j \geq l+1$.

Proof. It suffices to show that, here, the terms in $\mathsf{B}_{2l,j}$ depend on the first variable. This amounts to showing that, if $j \geq l+1$, $(k_i : 1 \leq i \leq 2l-j+1)$ satisfy (B.2) with $m = 2l$, then $k_1 \neq 0$. Indeed, let $(k_i : 1 \leq i \leq 2l-j+1)$ be non-negative integers such that (B.2) are satisfied but $k_1 = 0$. Then, $\sum k_i = j \geq l+1$ with $2 \leq i \leq 2l-j+1$. On the other hand, due to the second condition in (B.2) being true, we have

$$\sum_{i=2}^{2l-j+1} ik_i = \sum_{i=2}^{2l-j+1} (i-2)k_i + 2 \sum_{i=2}^{2l-j+1} k_i \geq 2(l+1) > 2l, \tag{B.4}$$

an evident contradiction. This, therefore, completes the proof. $\square$

C. Bounds on the derivatives of $\operatorname{tr} e^{t\Delta}$**.** Letting M be a complete Riemannian manifold, we recall that there exists a $c > 0$ such that

$$|\operatorname{tr} e^{z\Delta}| \leq c\Re(z)^{-n/2} \tag{C.1}$$

for all $\Re(z) > 0$. We also recall that the trace of the heat kernel is analytic in z for $\Re(z) > 0$. Let γ be the circle in $\mathbb{C}$ with center $s \in (0, \infty)$ and radius $s/2$. Then, if $z \in \gamma$, we have $s/2 \leq \Re(z) \leq 3s/2$. Therefore, using Cauchy's integral formula, we have

$$\begin{aligned} \left| \frac{d^j}{ds^j} \operatorname{tr} e^{s\Delta} \right| &= \left| \frac{1}{2\pi i} \oint_\gamma \frac{\operatorname{tr} e^{-z\Delta}}{(z-s)^{j+1}}\, dz \right| \\ &\leq \frac{c}{2\pi s^{j+1}} \oint_\gamma \Re(z)^{-n/2} dz \leq c\left(\frac{3}{2}\right)^{-n/2} s^{-n/2-j}. \end{aligned} \tag{C.2}$$

ENDNOTES

1. For more details on Gegenbauer polynomials and applications, see [**1, 26, 34**].

2. The coefficients of the Bell polynomials relate to the number of ways a given set can be partitioned, and thus, have many applications in combinatorics (cf., [**6**] for more details).

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