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Gaussian bounds for the heat kernels on the ball and the simplex: classical approach

by

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Abstract. Two-sided Gaussian bounds are established for the weighted heat kernels on the unit ball and the simplex in $\mathbb{R}^d$ generated by classical differential operators whose eigenfunctions are algebraic polynomials.

1. Introduction. Two-sided Gaussian bounds have been established for heat kernels in various settings. For example, Gaussian bounds for the Jacobi heat kernel on $[-1,1]$ with weight $(1-x)^\alpha(1+x)^\beta$, $\alpha,\beta > -1$, are obtained in [2, Theorem 7.2] and [8, Theorem 5.1], and also in [9] for $\alpha,\beta \geq -1/2$ (see (1.24) below).

In this article we establish two-sided Gaussian estimates for the heat kernels generated by classical differential operators whose eigenfunctions are algebraic polynomials in the weighted cases on the unit ball and the simplex in $\mathbb{R}^d$. Such estimates are also established in [8] using a general method that utilizes known two-sided Gaussian estimates for the heat kernels generated by weighted Laplace operators on Riemannian manifolds. Here we derive these results directly from the Gaussian bounds for the Jacobi heat kernel. Such a direct method leads to working in somewhat restricted range for the parameters of the weights (commonly used in the literature). More recently, another proof of the Gaussian bounds for the heat kernel on the ball appeared in [12]. We next describe our results in detail.

We shall use standard notation. In particular, positive constants will be denoted by $c, c', \tilde{c}, c_1, c_2, \ldots$ and they may vary at each occurrence. Most constants will depend on parameters that will be clear from the context.

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The notation $a \sim b$ will stand for $c_1 \le a/b \le c_2$. The functions that we deal with in this article are assumed to be real-valued.

1.1. Heat kernel on the unit ball. Consider the operator

$$\mathcal{D}_\mu := \sum_{i=1}^{d}(1-x_i^2)\partial_i^2 - 2\sum_{1\le i<j\le d} x_i x_j \partial_i\partial_j - (d+2\mu)\sum_{i=1}^{d} x_i\partial_i, \tag{1.1}$$

acting on sufficiently smooth functions on $\mathbb{B}^d := \{x \in \mathbb{R}^d : \|x\| < 1\}$, the unit ball in $\mathbb{R}^d$, equipped with the measure

$$d\nu_\mu = w_\mu(x)dx := (1-\|x\|^2)^{\mu-1/2}dx, \qquad \mu \ge 0, \tag{1.2}$$

and the distance

$$d_{\mathbb{B}}(x,y) := \arccos\big(\langle x,y\rangle + \sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big), \tag{1.3}$$

where $\langle x,y\rangle$ is the inner product of $x,y \in \mathbb{R}^d$ and $\|x\| := \sqrt{\langle x,x\rangle}$. As will be shown, the operator $\mathcal{D}_\mu$ is symmetric and $-\mathcal{D}_\mu$ is positive in $L^2(\mathbb{B}^d, w_\mu)$. Furthermore, $\mathcal{D}_\mu$ is essentially self-adjoint.

For $0 \le r \le 1$ denote

$$B_{\mathbb{B}}(x,r) := \{y \in \mathbb{R}^d : d_{\mathbb{B}}(x,y) < r\} \quad \text{and} \quad V_{\mathbb{B}}(x,r) := \nu_\mu(B_{\mathbb{B}}(x,r)). \tag{1.4}$$

As is well known (see e.g. [3, Lemma 11.3.6]),

$$V_{\mathbb{B}}(x,r) \sim r^d(1-\|x\|^2+r^2)^\mu. \tag{1.5}$$

Denote by $\mathcal{V}_n(w_\mu)$ the set of all algebraic polynomials of degree n in d variables that are orthogonal to lower degree polynomials in $L^2(\mathbb{B}^d, w_\mu)$, and let $\mathcal{V}_0(w_\mu)$ be the set of all constants. As is well known (see e.g. [5, §5.2]), $\mathcal{V}_n(w_\mu)$, $n = 0, 1, \dots$, are eigenspaces of the operator $\mathcal{D}_\mu$, more precisely,

$$\mathcal{D}_\mu P = -n(n+d+2\mu-1)P, \qquad \forall P \in \mathcal{V}_n(w_\mu). \tag{1.6}$$

Let $P_n(w_\mu; x, y)$ be the kernel of the orthogonal projector onto $\mathcal{V}_n(w_\mu)$. Then the semigroup $e^{t\mathcal{D}_\mu}$, $t > 0$, generated by $\mathcal{D}_\mu$ has a (heat) kernel $e^{t\mathcal{D}_\mu}(x,y)$ of the form

$$e^{t\mathcal{D}_\mu}(x,y) = \sum_{n=0}^{\infty} e^{-tn(n+2\lambda)}P_n(w_\mu; x, y), \qquad \lambda := \mu + (d-1)/2. \tag{1.7}$$

We establish two-sided Gaussian bounds on $e^{t\mathcal{D}_\mu}(x,y)$:

THEOREM 1.1. *For any $\mu \ge 0$ there exist constants $c_1, c_2, c_3, c_4 > 0$ such that for all $x, y \in \mathbb{B}^d$ and $t > 0$,*

$$\frac{c_1 \exp\{-\frac{d_{\mathbb{B}}(x,y)^2}{c_2 t}\}}{[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})]^{1/2}} \le e^{t\mathcal{D}_\mu}(x,y) \le \frac{c_3 \exp\{-\frac{d_{\mathbb{B}}(x,y)^2}{c_4 t}\}}{[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})]^{1/2}}. \tag{1.8}$$

1.2. Heat kernel on the simplex. We also establish two-sided Gaussian bounds for the heat kernel generated by the operator

$$\mathcal{D}_\kappa := \sum_{i=1}^d x_i\partial_i^2 - \sum_{i=1}^d\sum_{j=1}^d x_ix_j\partial_i\partial_j + \sum_{i=1}^d\big(\kappa_i + \tfrac12 - \big(|\kappa| + \tfrac{d+1}{2}\big)x_i\big)\partial_i \tag{1.9}$$

with $|\kappa| := \kappa_1 + \cdots + \kappa_{d+1}$ acting on sufficiently smooth functions on the simplex

$$\mathbb{T}^d := \{x \in \mathbb{R}^d : x_1 \ge 0, \dots, x_d \ge 0, |x| \le 1\}, \qquad |x| := x_1 + \cdots + x_d,$$

in $\mathbb{R}^d$, $d \ge 1$, equipped with the measure

$$d\nu_\kappa(x) = w_\kappa(x)dx := \prod_{i=1}^d x_i^{\kappa_i - 1/2}(1-|x|)^{\kappa_{d+1}-1/2}dx, \qquad \kappa_i \ge 0, \tag{1.10}$$

and the distance

$$d_{\mathbb{T}}(x,y) := \arccos\Big(\sum_{i=1}^d \sqrt{x_iy_i} + \sqrt{1-|x|}\sqrt{1-|y|}\Big). \tag{1.11}$$

As will be shown, the operator $\mathcal{D}_\kappa$ is symmetric and $-\mathcal{D}_\kappa$ is positive in the weighted space $L^2(\mathbb{T}, w_\kappa)$; furthermore, $\mathcal{D}_\kappa$ is essentially self-adjoint.

We shall use the notation

$$B_{\mathbb{T}}(x,r) := \{y \in \mathbb{T}^d : d_{\mathbb{T}}(x,y) < r\} \quad \text{and} \quad V_{\mathbb{T}}(x,r) := \nu_\kappa(B_{\mathbb{T}}(x,r)). \tag{1.12}$$

It is known that for $0 \le r \le 1$,

$$V_{\mathbb{T}}(x,r) \sim r^d(1-|x|+r^2)^{\kappa_{d+1}}\prod_{i=1}^d (x_i + r^2)^{\kappa_i}. \tag{1.13}$$

This equivalence follows e.g. from [3, (5.1.10)] (see also [8, (4.23)–(4.24)]).

Denote by $\mathcal{V}_n(w_\kappa)$ the set of all algebraic polynomials of degree n in d variables that are orthogonal to lower degree polynomials in $L^2(\mathbb{T}^d, w_\kappa)$, and let $\mathcal{V}_0(w_\kappa)$ be the set of all constants. As is well known (e.g. [5, §5.3]), $\mathcal{V}_n(w_\kappa)$, $n = 0, 1, \dots$, are eigenspaces of the operator $\mathcal{D}_\kappa$, namely,

$$\mathcal{D}_\kappa P = -n(n + |\kappa| + (d-1)/2)P, \qquad \forall P \in \mathcal{V}_n(w_\kappa),\ n = 0, 1, \dots. \tag{1.14}$$

Let $P_n(w_\kappa; x, y)$ be the kernel of the orthogonal projector onto $\mathcal{V}_n(w_\kappa)$ in $L^2(\mathbb{T}^d, w_\kappa)$. The heat kernel $e^{t\mathcal{D}_\kappa}(x,y)$, $t > 0$, takes the form

$$e^{t\mathcal{D}_\kappa}(x,y) = \sum_{n=0}^\infty e^{-tn(n+\lambda_\kappa)}P_n(w_\kappa; x, y), \qquad \lambda_\kappa := |\kappa| + (d-1)/2. \tag{1.15}$$

Theorem 1.2. *For any $\kappa_i \ge 0$, $i = 1, \dots, n+1$, there are constants $c_1, c_2, c_3, c_4 > 0$ such that for all $x, y \in \mathbb{T}^d$ and $t > 0$,*

$$\frac{c_1 \exp\big\{-\frac{d_{\mathbb{T}}(x,y)^2}{c_2 t}\big\}}{[V_{\mathbb{T}}(x,\sqrt t)V_{\mathbb{T}}(y,\sqrt t)]^{1/2}} \le e^{t\mathcal{D}_\kappa}(x,y) \le \frac{c_3 \exp\big\{-\frac{d_{\mathbb{T}}(x,y)^2}{c_4 t}\big\}}{[V_{\mathbb{T}}(x,\sqrt t)V_{\mathbb{T}}(y,\sqrt t)]^{1/2}}. \tag{1.16}$$

1.3. Method of proof and discussion. We shall prove Theorems 1.1 and 1.2 by using the known two-sided Gaussian bounds on the Jacobi heat kernel on $[-1,1]$. We next describe this result. The classical Jacobi operator is defined by

$$L_{\alpha,\beta}f(x) := \frac{[w_{\alpha,\beta}(x)(1-x^2)f'(x)]'}{w_{\alpha,\beta}(x)}, \tag{1.17}$$

where

$$w_{\alpha,\beta}(x) := (1-x)^\alpha(1+x)^\beta, \quad \alpha,\beta > -1.$$

We consider $L_{\alpha,\beta}$ with domain $D(L) := \mathcal{P}[-1,1]$ the set of all algebraic polynomials restricted to $[-1,1]$. We also consider $[-1,1]$ equipped with the weighted measure

$$d\nu_{\alpha,\beta}(x) := w_{\alpha,\beta}(x)dx = (1-x)^\alpha(1+x)^\beta dx \tag{1.18}$$

and the distance

$$\rho(x,y) := |\arccos x - \arccos y|. \tag{1.19}$$

It is not hard to see that the Jacobi operator $L_{\alpha,\beta}$ in the setting described above is essentially self-adjoint and $-L_{\alpha,\beta}$ is positive in $L^2([-1,1], w_{\alpha,\beta})$.

We shall use the notation

$$B(x,r) := \{y \in [-1,1] : \rho(x,y) < r\} \text{ and } V(x,r) := \nu_{\alpha,\beta}(B(x,r)). \tag{1.20}$$

As is well known (see e.g. [2, (7.1)]),

$$V(x,r) \sim r(1-x+r^2)^{\alpha+1/2}(1+x+r^2)^{\beta+1/2}, \quad x \in [-1,1],\ 0 < r \le \pi. \tag{1.21}$$

It is well known [13] that the Jacobi polynomials $P_n^{(\alpha,\beta)}$, $n = 0,1,\dots,$ are eigenfunctions of the operator $L_{\alpha,\beta}$, namely,

$$L_{\alpha,\beta}P_n^{(\alpha,\beta)} = -n(n+\alpha+\beta+1)P_n^{(\alpha,\beta)}, \quad n = 0,1,\dots. \tag{1.22}$$

The Jacobi polynomials $\{P_n^{(\alpha,\beta)}\}$ are standardly normalized by the condition $P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}$ [13]. As usual we denote $h_n^{(\alpha,\beta)} := \|P_n^{(\alpha,\beta)}\|^2_{L^2([-1,1],w_{\alpha,\beta})}$. Then the Jacobi heat kernel $e^{tL_{\alpha,\beta}}(x,y)$, $t>0$, takes the form

$$e^{tL_{\alpha,\beta}}(x,y) = \sum_{n=0}^\infty e^{-tn(n+\alpha+\beta+1)}\frac{P_n^{(\alpha,\beta)}(x)P_n^{(\alpha,\beta)}(y)}{h_n^{(\alpha,\beta)}}. \tag{1.23}$$

THEOREM 1.3. *For any $\alpha,\beta > -1$ there exist constants $c_1,c_2,c_3,c_4 > 0$ such that for all $x,y \in [-1,1]$ and $t > 0$,*

$$\frac{c_1\exp\{-\frac{\rho(x,y)^2}{c_2t}\}}{[V(x,\sqrt{t})V(y,\sqrt{t})]^{1/2}} \le e^{tL_{\alpha,\beta}}(x,y) \le \frac{c_3\exp\{-\frac{\rho(x,y)^2}{c_4t}\}}{[V(x,\sqrt{t})V(y,\sqrt{t})]^{1/2}}. \tag{1.24}$$

This theorem is established in [2, Theorem 7.2] using a general result on heat kernels in Dirichlet spaces with a doubling measure and a local

Poincaré inequality. The same theorem is also proved in [8, Theorem 5.1]. In [9] Nowak and Sjögren obtained this result in the case when $\alpha, \beta \geq -1/2$ via a direct method using special functions.

For the proof of Theorem 1.1 it will be critical that the kernel $P(w_\mu; x, y)$ of the orthogonal projector onto $\mathcal{V}_n(w_\mu)$ in $L^2(\mathbb{B}, w_\mu)$ has an explicit representation in terms of the univariate Gegenbauer polynomials (see (2.5)–(2.7)). For the proof of Theorem 1.2 we apply the well known representation of the kernel $P_n(w_\kappa; x, y)$ in terms of Jacobi polynomials (see (3.6)).

It should be pointed out that our method of proof of estimates (1.8) and (1.16) works only in the range $\mu \geq 0$ for the weight parameter in the case of the ball and in the range $\kappa_i \geq 0$, $i = 1, \dots, n$, in the case of the simplex. These restrictions on the range of the parameters are determined by the range for the parameters in the representations of the kernels $P(w_\mu; x, y)$ and $P_n(w_\kappa; x, y)$.

Observe that the two-sided estimates on the heat kernels from (1.8), (1.16) coupled with the general results from [2, 7] entail smooth functional calculus in the settings on the ball and the simplex (see [6, 11]), in particular, the finite speed propagation property is valid. For more details, see [8, §3.1].

2. Proof of Gaussian bounds for the heat kernel on the ball. We adhere to the notation from §1.1. Define

$$D_{i,j} := x_i \partial_j - x_j \partial_i, \qquad 1 \leq i \neq j \leq d.$$

It is easy to see that

$$D_{i,j} = \partial_{\theta_{i,j}} \quad \text{with} \quad (x_i, x_j) = r_{i,j}(\cos\theta_{i,j}, \sin\theta_{i,j}). \tag{2.1}$$

Further, define the second order differential operators

$$D_{i,i}^2 := [w_\mu(x)]^{-1} \partial_i [(1 - \|x\|^2) w_\mu(x) \partial_i], \qquad 1 \leq i \leq d.$$

It turns out that the differential operator $\mathcal{D}_\mu$ from (1.1) can be decomposed as a sum of second order differential operators [3, Proposition 7.1]:

$$\mathcal{D}_\mu = \sum_{i=1}^{d} D_{i,i}^2 + \sum_{1 \leq i < j \leq d} D_{i,j}^2 = \sum_{1 \leq i \leq j \leq d} D_{i,j}^2. \tag{2.2}$$

The basic properties of the operator $\mathcal{D}_\mu$ are given in

THEOREM 2.1. *For $f \in C^2(\mathbb{B}^d)$ and $g \in C^1(\mathbb{B}^d)$,*

$$\begin{aligned} &\int_{\mathbb{B}^d} \mathcal{D}_\mu f(x) g(x) w_\mu(x)\, dx \\ &= -\int_{\mathbb{B}^d} \Big[\sum_{i=1}^{d} \partial_i f(x) \partial_i g(x) (1 - \|x\|)^2 + \sum_{1 \leq i < j \leq d} D_{i,j} f(x) D_{i,j} g(x)\Big] w_\mu(x)\, dx. \end{aligned} \tag{2.3}$$

Consequently, the operator $\mathcal{D}_\mu$ is essentially self-adjoint and $-\mathcal{D}_\mu$ is positive in $L^2(\mathbb{B}^d, w_\mu)$.

Proof. Applying integration by parts in the variable x_i we obtain

$$\int_{\mathbb{B}^d} (D_{i,i}^2 f(x))g(x)w_\mu(x)\,dx = \int_{\mathbb{B}^d} \big(\partial_i[(1-\|x\|^2)w_\mu(x)\partial_i f(x)]\big)g(x)\,dx$$
$$= -\int_{\mathbb{B}^d} \partial_i f(x)\partial_i g(x)(1-\|x\|)^2 w_\mu(x)\,dx.$$

We now handle $D_{i,j}^2$. It is sufficient to consider $D_{1,2}$. If $d = 2$ we switch to polar coordinates and use (2.1) and integration by parts for 2π-periodic functions to obtain

$$\int_{\mathbb{B}^2} (D_{i,j}^2 f(x))g(x)w_\mu(x)\,dx = \int_0^1 r(1-r^2)^{\mu-1/2} \int_0^{2\pi} (\partial_\theta^2 f)g\,d\theta\,dr$$
$$= -\int_0^1 r(1-r^2)^{\mu-1/2} \int_0^{2\pi} \partial_\theta f \partial_\theta g\,d\theta\,dr$$
$$= -\int_{\mathbb{B}^2} D_{i,j} f(x) D_{i,j} g(x) w_\mu(x)\,dx.$$

In dimension $d > 2$ we apply the following integration identity that follows by a simple change of variables:

$$\int_{\mathbb{B}^d} f(x)\,dx = \int_{\mathbb{B}^{d-2}} \Big[\int_{\mathbb{B}^2} f\big(\sqrt{1-\|v\|^2}\,u, v\big)\,du\Big](1-\|v\|^2)\,dv, \tag{2.4}$$

and parametrizing the integral over $\mathbb{B}^2$ by polar coordinates we arrive at

$$\int_{\mathbb{B}^d} (D_{i,j}^2 f(x))g(x)w_\mu(x)\,dx = -\int_{\mathbb{B}^d} D_{i,j} f(x) D_{i,j} g(x) w_\mu(x)\,dx.$$

The above identities imply (2.3).

We consider the operator $\mathcal{D}_\mu$ with domain $D(\mathcal{D}_\mu) = \mathcal{P}(\mathbb{B}^d)$ the set of all polynomials on $\mathbb{B}^d$, which is obviously dense in $L^2(\mathbb{B}^d, w_\mu)$. From (2.3) it readily follows that $\mathcal{D}_\mu$ is symmetric and $-\mathcal{D}_\mu$ is positive.

We next show that $\mathcal{D}_\mu$ is essentially self-adjoint, i.e. its completion $\overline{\mathcal{D}}_\mu$ is self-adjoint. Let $\{P_{nj} : j = 1, \dots, \dim \mathcal{V}_n\}$ be an orthonormal basis of $\mathcal{V}_n = \mathcal{V}_n(w_\mu)$ consisting of real-valued polynomials. Clearly

$$D(\mathcal{D}_\mu) = \Big\{f = \sum_{n,j} a_{nj} P_{nj} : a_{nj} \in \mathbb{R},\ \{a_{nj}\} \text{ compactly supported}\Big\},$$
$$\mathcal{D}_\mu f = -\sum_{n,j} a_{nj} n(n+2\lambda) P_{nj} \quad \text{if} \quad f = \sum_j a_{nj} P_{nj} \in D(\mathcal{D}_\mu).$$

We define $\overline{\mathcal{D}}_\mu$ and its domain $D(\overline{\mathcal{D}}_\mu)$ by

$$D(\overline{\mathcal{D}}_\mu) := \Big\{ f = \sum_{n=0}^{\infty} \sum_{j=1}^{\dim \mathcal{V}_n} a_{nj} P_{nj} : \sum_{n,j} |a_{nj}|^2 < \infty, \\ \sum_{n,j} |a_{nj}|^2 (n(n+2\lambda))^2 < \infty \Big\}$$

and

$$\overline{\mathcal{D}}_\mu f := -\sum_{n,j} a_{nj} n(n+2\lambda) P_{nj} \quad \text{if} \quad f = \sum_{n,j} a_{nj} P_{nj} \in D(\overline{\mathcal{D}}_\mu).$$

It is easy to show that $\overline{\mathcal{D}}_\mu$ is the closure of $\mathcal{D}_\mu$ and that $\overline{\mathcal{D}}_\mu$ is self-adjoint. ∎

REMARK 2.2. Identity (2.3) is the weighted Green formula on $\mathbb{B}^d$ (see [8]).

Proof of Theorem 1.1. We shall assume that $0 < t \le 1$. For $t > 1$ the Gaussian bounds (1.8) obviously follow from (1.8) with $t = 1$.

It is known (see [5, Thm. 5.2.8]) that for $\mu > 0$ the kernel $P_n(w_\mu; x, y)$ of the orthogonal projector onto $\mathcal{V}_n(w_\mu)$ in $L^2(\mathbb{B}, w_\mu)$ has the representation

$$\tag{2.5} P_n(w_\mu; x, y) \\ = c_\mu \frac{n+\lambda}{\lambda} \int_{-1}^{1} C_n^\lambda\big(\langle x, y\rangle + u\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big)(1-u^2)^{\mu-1}\, du,$$

where C_n^λ is the Gegenbauer polynomial of degree n, and c_μ is the constant such that $c_\mu \int_{-1}^1 (1-t^2)^{\mu-1} dt = 1$. The Gegenbauer polynomials $\{C_n^\lambda\}$ are orthogonal in the weighted space $L^2([-1,1], w_\lambda)$ with $w_\lambda(u) := (1-u^2)^{\lambda-1/2}$ and can be defined by the generating function

$$(1-2uz+z^2)^{-\lambda} = \sum_{n=0}^{\infty} C_n^\lambda(u) z^n, \qquad |z|, |u| < 1.$$

Using $C_n^\lambda(1) = \binom{n+2\lambda-1}{n}$ it is easy to show that

$$\tag{2.6} c_{\lambda+1/2} \int_{-1}^{1} |C_n^\lambda(u)|^2 w_\lambda(u)\, du = \frac{\lambda}{n+\lambda} C_n^\lambda(1).$$

In the limiting case $\mu = 0$ the representation of $P_n(w_\mu; x, y)$ takes the form

$$\tag{2.7} P_n(w_0; x, y) = \frac{\lambda+n}{\lambda}\big[C_n^\lambda\big(\langle x, y\rangle + \sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big) \\ + C_n^\lambda\big(\langle x, y\rangle - \sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big)\big].$$

If $\alpha = \beta = \lambda - 1/2$, we denote the Jacobi operator by $L_\lambda := L_{\lambda-1/2,\lambda-1/2}$ and we have $L_\lambda f(x) = (1-x^2) f''(x) - (2\lambda+1) f'(x)$. We denote by $e^{tL_\lambda}(u, v)$

the associated Jacobi heat kernel. By (1.23) and (2.6) we obtain
(2.8)
$$e^{tL_\lambda}(u,v)=\sum_{n=0}^{\infty}e^{-tn(n+2\lambda)}\frac{c_{\lambda+1/2}(n+\lambda)}{\lambda}\frac{C_n^\lambda(u)C_n^\lambda(v)}{C_n^\lambda(1)},\qquad \lambda:=\mu+(d-1)/2.$$

Assume $\mu>0$. The above, (1.7), and (2.5) lead to the representation

$$e^{t\mathcal{D}_\mu}(x,y)=\frac{c_\mu}{c_{\lambda+1/2}}\int_{-1}^{1}e^{tL_\lambda}\big(1,\langle x,y\rangle+u\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big)(1-u^2)^{\mu-1}\,du. \tag{2.9}$$

Note that in the case of Gegenbauer polynomials ($\alpha=\beta=\lambda-1/2$) by (1.21) it follows that $V(x,r)\sim r(1-x^2+r^2)^\lambda$, $-1\le x\le 1$, and hence

$$V(1,\sqrt{t})\sim t^{\lambda+1/2},\quad V(z,\sqrt{t})\sim t^{\lambda+1/2}(1+(1-z^2)/t)^\lambda,\quad |z|\le 1. \tag{2.10}$$

If $x=\cos\theta$, then $1-x=2\sin^2(\theta/2)\sim\theta^2$ and hence

$$\rho(1,z)=|\arccos 1-\arccos z|=\arccos z\sim\sqrt{1-z},\qquad -1\le z\le 1. \tag{2.11}$$

From this, (2.9), (1.24), and (2.10) we obtain

$$e^{t\mathcal{D}_\mu}(x,y)\le c_1\int_{-1}^{1}\frac{\exp\{-\frac{1-z(u;x,y)}{c_2t}\}}{t^{\lambda+1/2}\big(1+\frac{1-z(u;x,y)^2}{t}\big)^{\lambda/2}}(1-u^2)^{\mu-1}\,du, \tag{2.12}$$

$$e^{t\mathcal{D}_\mu}(x,y)\ge c_3\int_{-1}^{1}\frac{\exp\{-\frac{1-z(u;x,y)}{c_4t}\}}{t^{\lambda+1/2}\big(1+\frac{1-z(u;x,y)^2}{t}\big)^{\lambda/2}}(1-u^2)^{\mu-1}\,du, \tag{2.13}$$

where $z(u;x,y):=\langle x,y\rangle+u\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}$.

Since $1+b\le e^b$ for $b\ge 0$, we have

$$1\le\Big(1+\frac{1-z^2}{t}\Big)^{\lambda/2}\le\Big(1+2\frac{1-z}{t}\Big)^{\lambda/2}\le\exp\Big\{\lambda\frac{1-z}{t}\Big\},\qquad |z|\le 1.$$

Therefore, by replacing the constant c_4 in (2.13) by a smaller constant c_4' we get

$$e^{t\mathcal{D}_\mu}(x,y)\ge\frac{c_3'}{t^{\lambda+1/2}}\int_{-1}^{1}\exp\Big\{-\frac{1-z(u;x,y)}{c_4't}\Big\}(1-u^2)^{\mu-1}\,du. \tag{2.14}$$

Obviously, from (2.12) it follows that

$$e^{t\mathcal{D}_\mu}(x,y)\le\frac{c_1}{t^{\lambda+1/2}}\int_{-1}^{1}\exp\Big\{-\frac{1-z(u;x,y)}{c_2t}\Big\}(1-u^2)^{\mu-1}\,du. \tag{2.15}$$

We have

$$1 - z(u;x,y) = 1 - \langle x,y\rangle - \sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2} + (1-u)\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}$$

and using the definition of $d_{\mathbb{B}}(x,y)$ in (1.3) we get

$$1 - z(1;x,y) = 1 - \cos d_{\mathbb{B}}(x,y) = 2\sin^2\frac{d_{\mathbb{B}}(x,y)}{2} \sim d_{\mathbb{B}}(x,y)^2.$$

Hence,

$$1-z(u;x,y) \sim d_{\mathbb{B}}(x,y)^2 + (1-u)H(x,y), \quad H(x,y) := \sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}.$$

Consequently,

$$\exp\Big\{-\frac{1-z(u;x,y)}{c_2 t}\Big\} \le \exp\Big\{-\frac{d_{\mathbb{B}}(x,y)^2}{c't}\Big\}\exp\Big\{-\frac{(1-u)H(x,y)}{c't}\Big\},$$

$$\exp\Big\{-\frac{1-z(u;x,y)}{2c_4 t}\Big\} \ge \exp\Big\{-\frac{d_{\mathbb{B}}(x,y)^2}{c''t}\Big\}\exp\Big\{-\frac{(1-u)H(x,y)}{c''t}\Big\}.$$

These two inequalities along with (2.14)–(2.15) imply that in order to obtain the two-sided Gaussian bounds in (1.8) it suffices to show that the quantity

$$A_t(x,y) := \frac{1}{t^{\lambda+1/2}}\int_{-1}^{1}\exp\Big\{-\frac{(1-u)H(x,y)}{ct}\Big\}(1-u^2)^{\mu-1}\,du \tag{2.16}$$

satisfies the following inequalities, for any $\varepsilon > 0$:

$$\frac{c^\star}{[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})]^{1/2}} \le A_t(x,y) \le \frac{c^{\star\star}\exp\{\varepsilon\frac{d_{\mathbb{B}}(x,y)^2}{t}\}}{[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})]^{1/2}}. \tag{2.17}$$

Here the constant $c^{\star\star} > 0$ depends on ε.

Lower bound. First, assume that $H(x,y)/t \ge 1$. Then

$$\begin{aligned} A_t(x,y) &\ge \frac{\tilde{c}}{t^{\lambda+1/2}}\int_0^1\exp\Big\{-\frac{(1-u)H(x,y)}{ct}\Big\}(1-u)^{\mu-1}\,du \\ &= \frac{\tilde{c}t^\mu}{t^{\lambda+1/2}H(x,y)^\mu}\int_0^{H(x,y)/t} v^{\mu-1}e^{-v/c}\,dv \\ &\ge \frac{c_*}{t^{d/2}H(x,y)^\mu} \quad \text{with} \quad c_* = \tilde{c}\int_0^1 v^{\mu-1}e^{-v/c}\,dv, \end{aligned} \tag{2.18}$$

where we have applied the substitution $v = (1-u)H(x,y)/t$ and used $\lambda + 1/2 = \mu + d/2$. However, by (1.5), $V_{\mathbb{B}}(x,r) \ge cr^d(1-\|x\|^2)^\mu$, which implies

$$t^{d/2}H(x,y)^\mu = t^{d/2}\big(\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big)^\mu \le \big[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t}\big]^{1/2}.$$

Putting the above together we conclude that $A_t(x,y)$ obeys the lower bound in (2.17) in this case.

Now, assume that $H(x,y)/t \le 1$. Then $\exp\{-\frac{(1-u)H(x,y)}{ct}\} \ge e^{-1/c}$ and

$$A_t(x,y) \ge \frac{\tilde{c}}{t^{\lambda+1/2}} \ge \frac{c^\star}{[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})]^{1/2}}.$$

Here we have used the fact that, by (1.5), $V_{\mathbb{B}}(x,r) \ge cr^{d+2\mu} = cr^{2\lambda+1}$. Thus, $A_t(x,y)$ again obeys the lower bound in (2.17) and this completes its proof.

Upper bound. Obviously $\exp\{-\frac{(1-u)H(x,y)}{ct}\} \le 1$ and hence

$$A_t(x,y) \le \frac{c_*}{t^{\lambda+1/2}} = \frac{c_*}{t^{d/2+\mu}}. \tag{2.19}$$

We shall obtain another estimate on $A_t(x,y)$ by breaking the integral in (2.16) into two parts: over $[0,1]$ and over $[-1,0]$. Just as in (2.18) applying the substitution $v = (1-u)H(x,y)/t$ we obtain

$$\frac{1}{t^{\lambda+1/2}}\int_0^1 \exp\Big\{-\frac{(1-u)H(x,y)}{ct}\Big\}(1-u^2)^{\mu-1}\,du \le \frac{c^*\max\{1,2^{\mu-1}\}}{t^{d/2}H(x,y)^\mu}$$

with $c^* = \int_0^\infty v^{\mu-1}e^{-v/c}\,dv$. Here we have used $(1+u)^{\mu-1} \le \max\{1,2^{\mu-1}\}$.

For the integral over $[-1,0]$ we use the fact that $1-u \ge 1$ for $u \in [-1,0]$ to obtain

$$\begin{aligned}\frac{1}{t^{\lambda+1/2}}&\int_{-1}^0 \exp\Big\{-\frac{(1-u)H(x,y)}{ct}\Big\}(1-u^2)^{\mu-1}\,du\\ &\le \frac{c_*}{t^{\lambda+1/2}}\exp\Big\{-\frac{H(x,y)}{ct}\Big\} \le \frac{\tilde{c}}{t^{\lambda+1/2}}\Big(\frac{t}{H(x,y)}\Big)^\mu = \frac{\tilde{c}}{t^{d/2}H(x,y)^\mu}.\end{aligned}$$

Here we have used $v^\mu \le \lfloor \mu+1 \rfloor! e^v$ for all $v>0$, and $\lambda = \mu + (d-1)/2$.

Together, the above inequalities imply

$$A_t(x,y) \le \frac{c^*}{t^{d/2}H(x,y)^\mu}. \tag{2.20}$$

In turn, (2.19) and (2.20) yield

$$A_t(x,y) \le \frac{c_\diamond}{t^{d/2}(t+H(x,y))^\mu}. \tag{2.21}$$

It remains to show that the above estimate implies the upper bound in (2.17). To this end we need the following simple inequalities:

$$(u+a)(u+b) \le 3(u^2+ab)(1+u^{-1}|a-b|), \qquad a,b \ge 0,\ 0<u\le 1 \tag{2.22}$$

(see, e.g. [10, (2.21)]) and (see [11, (4.9)])

$$\big|\sqrt{1-\|x\|^2} - \sqrt{1-\|y\|^2}\big| \le \sqrt{2}\, d_{\mathbb{B}}(x,y), \qquad x,y \in \mathbb{B}^d.$$

Together, these two inequalities yield

$$(2.23)\qquad \big(\sqrt{t}+\sqrt{1-\|x\|^2}\big)\big(\sqrt{t}+\sqrt{1-\|y\|^2}\big) \le c\big(t+H(x,y)\big)\left(1+\frac{d_{\mathbb{B}}(x,y)}{\sqrt{t}}\right).$$

Evidently $1+u \le \varepsilon^{-1}e^{\varepsilon u}$ for $u \ge 0$ and $0<\varepsilon\le 1$, and hence

$$(2.24)\qquad (1+b)^{\mu} \le 2^{\mu}(1+b^2)^{\mu/2} \le 2^{\mu}\varepsilon^{-\mu/2}e^{\mu\varepsilon b^2}, \qquad \forall b\ge 0,\ 0<\varepsilon\le 1.$$

Also, from (1.5) it follows that $V_{\mathbb{B}}(x,r) \sim r^d(r+\sqrt{1-\|x\|^2})^{2\mu}$. From this, (2.23), and (2.24) it follows that

$$\begin{aligned}\big[V_{\mathbb{B}}(x,\sqrt{t})V_{\mathbb{B}}(y,\sqrt{t})\big]^{1/2} &\le ct^{d/2}\big(\sqrt{t}+\sqrt{1-\|x\|^2}\big)^{\mu}\big(\sqrt{t}+\sqrt{1-\|y\|^2}\big)^{\mu}\\ &\le c_{\varepsilon}t^{d/2}(t+H(x,y))^{\mu}\exp\left\{\mu\varepsilon\frac{d_{\mathbb{B}}(x,y)^2}{t}\right\}.\end{aligned}$$

In turn, this and (2.21) yield the upper estimate in (2.17).

We next consider the case when $\mu=0$. Now, (1.7), (2.7), and (2.8) yield the representation

$$(2.25)\qquad \begin{aligned}e^{t\mathcal{D}_0}(x,y) &= c_{\lambda}e^{tL_{\lambda}}\big(1,\langle x,y\rangle+\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big)\\ &\quad + c_{\lambda}e^{tL_{\lambda}}\big(1,\langle x,y\rangle-\sqrt{1-\|x\|^2}\sqrt{1-\|y\|^2}\big).\end{aligned}$$

From this point on the proof follows in the footsteps of the proof when $\mu>0$ above, but is much simpler because the integral in (2.9) is replaced in (2.25) by two terms. We omit the further details. The proof of Theorem 1.1 is complete. ■

3. Proof of Gaussian bounds for the heat kernel on the simplex. In this part we adhere to the notation from §1.2. The differential operator $\mathcal{D}_{\kappa}$ from (1.9) can be represented in the more symmetric form

$$(3.1)\qquad \mathcal{D}_{\kappa} = \sum_{i=1}^{d} U_i + \sum_{1\le i<j\le d} U_{i,j},$$

where

$$\begin{aligned}U_i &:= \frac{1}{w_k(x)}\partial_i\big(x_i(1-|x|)w_{\kappa}(x)\partial_i\big),\\ U_{i,j} &:= \frac{1}{w_k(x)}(\partial_i-\partial_j)[x_ix_jw_{\kappa}(x)(\partial_i-\partial_j)], \qquad 1\le i<j\le d.\end{aligned}$$

This decomposition was first established in [1] for $w_{\kappa}(x)=1$ and later used in [4] with general w_{κ}. It is easy to verify it directly.

The following basic property of the operator $\mathcal{D}_{\kappa}$ follows from (3.1) by integration by parts:

Proposition 3.1. *For any* $f \in C^2(\mathbb{T}^d)$ *and* $g \in C^1(\mathbb{T}^d)$,

$$\int_{\mathbb{T}^d} \mathcal{D}_\kappa f(x) \cdot g(x) w_\kappa(x)\,dx = -\int_{\mathbb{T}^d} \Big[\sum_{i=1}^d \partial_i f(x)\partial_i g(x) x_i(1-|x|) + \sum_{1\le i<j\le d} (\partial_i - \partial_j) f(x)(\partial_i - \partial_j) g(x) x_i x_j\Big] w_\kappa(x)\,dx. \tag{3.2}$$

Proof. Fix $f \in C^2(\mathbb{T}^d)$ and $g \in C^1(\mathbb{T}^d)$. For any $x = (x_1, \dots, x_d)$ in $\mathbb{R}^d$ we denote $\hat{x}_i := (x_1, \dots, x_{i-1}, x_{i+1}, x_d) \in \mathbb{R}^{d-1}$. We use the identity

$$\int_{\mathbb{T}^d} h(x)\,dx = \int_{\mathbb{T}^{d-1}} \int_0^{1-|\hat{x}_i|} h(x)\,dx_i\,d\hat{x}_i \tag{3.3}$$

and integration by parts to obtain

$$\begin{aligned}\int_{\mathbb{T}^d} U_i f(x) \cdot g(x) w_\kappa(x)\,dx &= \int_{\mathbb{T}^d} \partial_i[x_i(1-|x|) w_\kappa(x) \partial_i f(x)] g(x)\,dx \\ &= \int_{\mathbb{T}^{d-1}} \Big[x_i(1-|x|) w_\kappa(x) \partial_i f(x) g(x)\Big|_{x_i=0}^{1-|\hat{x}_i|} \\ &\quad - \int_0^{1-|\hat{x}_i|} x_i(1-|x|) w_\kappa(x) \partial_i f(x) \partial_i g(x)\,dx_i\Big]\,d\hat{x}_i.\end{aligned}$$

Now, since $x_i(1-|x|)w_\kappa(x)$ vanishes when $x_i = 0$ or $x_i = 1 - |\hat{x}_i|$ we get

$$\int_{\mathbb{T}^d} U_i f(x) \cdot g(x) w_\kappa(x)\,dx = -\int_{\mathbb{T}^d} \partial_i f(x) \partial_i g(x) x_i(1-|x|) w_\kappa(x)\,dx. \tag{3.4}$$

We next show that

$$\int_{\mathbb{T}^d} U_{i,j} f(x) \cdot g(x) w_\kappa(x)\,dx = -\int_{\mathbb{T}^d} (\partial_i - \partial_j) f(x) \cdot (\partial_i - \partial_j) g(x) x_i x_j w_\kappa(x)\,dx. \tag{3.5}$$

For any $x = (x_1, \dots, x_d)$ we set

$$\xi_i(x) := (x_1, \dots, x_{i-1}, 1 - |\hat{x}_i|, x_{i+1}, \dots x_d).$$

Also, denote $F_{ij}(x) := (\partial_i - \partial_j) f(x)$.

Assume first that $\kappa_{d+1} > 1/2$. Just as above using (3.3) and integration by parts in x_i, we obtain

$$\begin{aligned}&\int_{\mathbb{T}^d} \partial_i[x_i x_j \omega_\kappa(x) F_{ij}(x)] \cdot g(x)\,dx \\ &= \int_{\mathbb{T}^{d-1}} \Big[x_i x_j \omega_\kappa(x) F_{ij}(x) g(x)\Big|_{x_i=0}^{1-|\hat{x}_i|} - \int_0^{1-|\hat{x}_i|} x_i x_j \omega_\kappa(x) F_{ij}(x) \partial_i g(x)\,dx_i\Big]\,d\hat{x}_i\end{aligned}$$

$$= \int_{\mathbb{T}^{d-1}} (1-|\hat{x}_i|)x_j\omega_\kappa(\xi_i(x))F_{ij}(\xi_i(x))g(\xi_i(x))\,dx$$
$$- \int_{\mathbb{T}^d} x_ix_j\omega_\kappa(x)F_{ij}(x)\cdot\partial_i g(x)\,dx = -\int_{\mathbb{T}^d} x_ix_j\omega_\kappa(x)F_{ij}(x)\cdot\partial_i g(x)\,dx.$$

Here we have used the fact that $x_i\omega_\kappa(x) = 0$ when $x_i = 0$ and $\omega_\kappa(\xi_i(x)) = 0$ since $\kappa_{d+1} > 1/2$. Similarly,

$$\int_{\mathbb{T}^d} \partial_j[x_ix_j\omega_\kappa(x)F_{ij}(x)]\cdot g(x)\,dx = -\int_{\mathbb{T}^d} x_ix_j\omega_\kappa(x)F_{ij}(x)\cdot\partial_j g(x)\,dx.$$

Subtracting the above identities proves (3.5) when $\kappa_{d+1} > 1/2$. The validity of (3.5) for all $\kappa_{d+1} > -1/2$ follows by analytic continuation in κ_{d+1}.

In light of (3.1), summing up (3.4) and (3.5) leads to (3.2). ∎

Observe that identity (3.2) is the weighted Green formula on the simplex $\mathbb{T}^d$ (see [8]).

We consider the operator $\mathcal{D}_\kappa$ defined on the set $D(\mathcal{D}_\kappa) = \mathcal{P}(\mathbb{T}^d)$ of all algebraic polynomials on $\mathbb{T}^d$, which is obviously dense in $L^2(\mathbb{T}^d, w_\kappa)$. From (3.2) it readily follows that $\mathcal{D}_\kappa$ is symmetric and $-\mathcal{D}_\kappa$ is positive in $L^2(\mathbb{T}^d, w_\kappa)$. Furthermore, just as in the proof of Theorem 2.1 it follows that $\mathcal{D}_\kappa$ is essentially self-adjoint.

Proof of Theorem 1.2. We may assume that $0 < t \le 1$, because the case $t > 1$ follows immediately from the case $t = 1$.

Recall that the Jacobi polynomials $\{P_n^{(\alpha,\beta)}\}$ are standardly normalized by $P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}$ and $h_n^{(\alpha,\beta)} = \|P_n^{(\alpha,\beta)}\|^2_{L^2([-1,1],w_{\alpha,\beta})}$. It is known (see [5, Theorem 5.3.4]) that if $\kappa_i > 0$ for all i, the kernel $P_n(w_\mu; x, y)$ of the orthogonal projector onto $\mathcal{V}_n(w_\kappa)$ in $L^2(\mathbb{T}^d, w_\kappa)$ has the following representation:

$$P_n(w_\mu; x, y) = c_\kappa (h_n^{(\lambda-1/2,-1/2)})^{-1} P_n^{(\lambda-1/2,-1/2)}(1) \times \int_{[-1,1]^{d+1}} P_n^{(\lambda-1/2,-1/2)}(2z(u; x, y)^2 - 1)\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du, \tag{3.6}$$

where

$$z(u; x, y) := \sum_{i=1}^{d+1} u_i\sqrt{x_iy_i},\ \ x_{d+1} := 1-|x|,\ \ y_{d+1} := 1-|y|,\ \ \lambda := |\kappa|+(d-1)/2,$$

with $|x| = x_1 + \cdots + x_d$. When some or all κ_i are 0, this identity holds in the limit $\kappa_i \to 0$, which can be shown using

$$\lim_{\kappa\to 0+} \frac{\int_{-1}^1 f(x)(1-x^2)^{\kappa-1}\,dx}{\int_{-1}^1 (1-x^2)^{\kappa-1}\,dx} = \frac{1}{2}[f(1) + f(-1)].$$

Assume $\kappa_i > 0$, $i = 1, \dots, n+1$. Combining (1.15), (1.23), and (3.6) we obtain the representation

$$(3.7)\qquad e^{t\mathcal{D}_\kappa}(x,y) = c_\kappa \int\limits_{[-1,1]^{d+1}} e^{tL_{\lambda-1/2,-1/2}}(1, 2z(u;x,y)^2-1)\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du.$$

Note that from the definition of the distance $d_{\mathbb{T}}(x,y)$ in (1.11) we have $\sum_{i=1}^{d+1}\sqrt{x_iy_i} = \cos d_{\mathbb{T}}(x,y)$ and hence $|z(u;x,y)| \le 1$. Just as in (2.11) we obtain

$$(3.8)\qquad \rho(1, 2z^2-1) := |\arccos 1 - \arccos(2z^2-1)| \sim \sqrt{1-(2z^2-1)} \sim \sqrt{1-z^2}.$$

On the other hand, with $\alpha = \lambda - 1/2$ and $\beta = -1/2$ we infer from (1.21) that $V(x,r) \sim r(1-x+r^2)^\lambda$ and hence $V(1,\sqrt{t}) \sim t^{\lambda+1/2}$ and

$$V(2z^2-1,\sqrt{t}) \sim t^{1/2}\big(t+2(1-z^2)\big)^\lambda \sim t^{\lambda+1/2}\Big(1+\frac{1-z^2}{t}\Big)^\lambda.$$

We use these equivalences, (3.7), (1.24), and (3.8) to obtain

$$(3.9)\qquad e^{t\mathcal{D}_\kappa}(x,y) \le c_1 \int\limits_{[-1,1]^{d+1}} \frac{\exp\big\{-\frac{1-z(u;x,y)^2}{c_2t}\big\}}{t^{\lambda+1/2}\big(1+\frac{1-z(u;x,y)^2}{t}\big)^{\lambda/2}}\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du,$$

$$(3.10)\qquad e^{t\mathcal{D}_\kappa}(x,y) \ge c_3 \int\limits_{[-1,1]^{d+1}} \frac{\exp\big\{-\frac{1-z(u;x,y)^2}{c_4t}\big\}}{t^{\lambda+1/2}\big(1+\frac{1-z(u;x,y)^2}{t}\big)^{\lambda/2}}\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du.$$

Just as in the proof of Theorem 1.1 by replacing the constant c_4 in (3.10) by a smaller constant c_4' we can eliminate the term $\big(1+\frac{1-z(u;x,y)^2}{t}\big)^\lambda$ in the denominator. Thus, it follows that

$$(3.11)\qquad e^{t\mathcal{D}_\kappa}(x,y) \ge \frac{c_3'}{t^{\lambda+1/2}} \int\limits_{[-1,1]^{d+1}} \exp\Big\{-\frac{1-z(u;x,y)^2}{c_4't}\Big\}\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du.$$

By simply deleting that term in (3.9) we get

$$e^{t\mathcal{D}_\kappa}(x,y) \le \frac{c_1}{t^{\lambda+1/2}} \int\limits_{[-1,1]^{d+1}} \exp\Big\{-\frac{1-z(u;x,y)^2}{c_2t}\Big\}\prod_{i=1}^{d+1}(1-u_i^2)^{\kappa_i-1}\,du.$$

Evidently,

$$1 - z(u;x,y)^2 = (1 + |z(u;x,y)|)(1 - |z(u;x,y)|) \geq 1 - |z(u,x,y)| \geq 1 - \sum_{i=1}^{d+1} |u_i|\sqrt{x_i y_i}.$$

Using the symmetry of the last term above with respect to sign changes of u_i, and the fact that $1 - u_i^2 \sim 1 - u_i$ when $0 \leq u_i \leq 1$, we conclude that

$$e^{t\mathcal{D}_\kappa}(x,y) \leq \frac{c_1'}{t^{\lambda+1/2}} \int_{[0,1]^{d+1}} \exp\left\{-\frac{1 - z(u;x,y)}{c_2 t}\right\} \prod_{i=1}^{d+1} (1 - u_i)^{\kappa_i - 1}\, du. \tag{3.12}$$

Similarly, using $1 - z(u;x,y)^2 \leq 2(1 - z(u;x,y))$ we infer from (3.11) that

$$e^{t\mathcal{D}_\kappa}(x,y) \geq \frac{c_3''}{t^{\lambda+1/2}} \int_{[0,1]^{d+1}} \exp\left\{-\frac{1 - z(u;x,y)}{c_4'' t}\right\} \prod_{i=1}^{d+1} (1 - u_i)^{\kappa_i - 1}\, du. \tag{3.13}$$

By the definition of $d_{\mathbb{T}}(x,y)$ in (1.11) we have

$$1 - \sum_{i=1}^{d+1} \sqrt{x_i y_i} = 1 - \cos d_{\mathbb{T}}(x,y) = 2\sin^2 \frac{d_{\mathbb{T}}(x,y)}{2} \sim d_{\mathbb{T}}(x,y)^2$$

and hence

$$\begin{aligned} 1 - z(u;x,y) &= 1 - \sum_{i=1}^{d+1} \sqrt{x_i y_i} + \sum_{i=1}^{d+1} (1 - u_i)\sqrt{x_i y_i} \\ &\sim d_{\mathbb{T}}(x,y)^2 + \sum_{i=1}^{d+1} (1 - u_i)\sqrt{x_i y_i}. \end{aligned} \tag{3.14}$$

Consequently,

$$\exp\left\{-\frac{1 - z(u;x,y)}{c_2 t}\right\} \leq \exp\left\{-\frac{d_{\mathbb{T}}(x,y)^2}{c' t}\right\} \prod_{i=1}^{d+1} \exp\left\{-\frac{(1 - u_i)\sqrt{x_i y_i}}{c' t}\right\}, \tag{3.15}$$

$$\exp\left\{-\frac{1 - z(u;x,y)}{c_4'' t}\right\} \geq \exp\left\{-\frac{d_{\mathbb{T}}(x,y)^2}{c'' t}\right\} \prod_{i=1}^{d+1} \exp\left\{-\frac{(1 - u_i)\sqrt{x_i y_i}}{c'' t}\right\}. \tag{3.16}$$

For $x, y \in [0,1]$ and $\kappa > 0$, denote

$$A_t(\kappa; x, y) := \kappa \int_0^1 \exp\left\{-\frac{(1 - u)\sqrt{xy}}{ct}\right\} (1 - u)^{\kappa - 1}\, du, \tag{3.17}$$

where $c>0$ is a constant. We claim that for any $0<\varepsilon\le 1$,

$$\frac{c_\diamond t^{|\kappa|}}{\prod_{i=1}^{d+1}(x_i+t)^{\kappa_i/2}(y_i+t)^{\kappa_i/2}} \le \prod_{i=1}^{d+1} A_t(\kappa_i;x_i,y_i) \le \frac{c^\diamond t^{|\kappa|}\exp\{\varepsilon\frac{d_{\mathbb{T}}(x,y)^2}{t}\}}{\prod_{i=1}^{d+1}(x_i+t)^{\kappa_i/2}(y_i+t)^{\kappa_i/2}}, \tag{3.18}$$

where $c^\diamond>0$ depends on ε.

Assume for a moment that the inequalities (3.18) are valid. Then by (3.12), (3.15), and the first inequality in (3.18) we obtain

$$\begin{aligned} e^{t\mathcal{D}_\kappa}(x,y) &\le \frac{c}{t^{|\kappa|+d/2}}\exp\Big\{-\frac{d_{\mathbb{T}}(x,y)^2}{c't}\Big\}\frac{t^{|\kappa|}\exp\{\varepsilon\frac{d_{\mathbb{T}}(x,y)^2}{t}\}}{\prod_{i=1}^{d+1}(x_i+t)^{\kappa_i/2}\prod_{i=1}^{d+1}(y_i+t)^{\kappa_i/2}} \\ &\le \frac{c\exp\{-\frac{d_{\mathbb{T}}(x,y)^2}{2c't}\}}{\big[V_{\mathbb{T}}(x,\sqrt{t})V_{\mathbb{T}}(y,\sqrt{t})\big]^{1/2}}. \end{aligned}$$

Here we have used the facts that $\lambda=|\kappa|+(d-1)/2$, and $V_{\mathbb{T}}(x,\sqrt{t})\sim t^{d/2}\prod_{i=1}^{d+1}(x_i+t)^{\kappa_i}$ and a similar expression for $V_{\mathbb{T}}(y,\sqrt{t})$. These follow readily from (1.13) since $x_{d+1}=1-|x|$. We have also used the second estimate in (3.18) with $\varepsilon=(2c')^{-1}$. The above inequalities yield the upper estimate in (1.16). One similarly shows that (3.13), (3.16), and the first inequality in (3.18) imply the lower estimate in (1.16).

It remains to prove the estimates in (3.18). We first focus on the lower estimate. If $\sqrt{xy}/t\le 1$, then $\exp\{-\frac{(1-u)\sqrt{xy}}{ct}\}\ge c'>0$ and hence

$$A_t(\kappa;x,y)\ge c'\ge\frac{c'}{(x/t+1)^{\kappa/2}(y/t+1)^{\kappa/2}}=\frac{c't^\kappa}{(x+t)^{\kappa/2}(y+t)^{\kappa/2}}.$$

Assume $\sqrt{xy}/t>1$. Then applying the substitution $v=(1-u)\sqrt{xy}/t$ we obtain

$$\begin{aligned} A_t(\kappa;x,y) &= \frac{\kappa t^\kappa}{(\sqrt{xy})^\kappa}\int_0^{\sqrt{xy}/t} e^{-v/c}v^{\kappa-1}\,dv \\ &\ge \frac{\kappa t^\kappa}{(\sqrt{xy})^\kappa}\int_0^1 e^{-v/c}v^{\kappa-1}\,dv = \frac{c''t^\kappa}{(\sqrt{xy})^\kappa}. \end{aligned}$$

Therefore, in both cases

$$A_t(\kappa;x,y)\ge\frac{ct^\kappa}{(x+t)^{\kappa/2}(y+t)^{\kappa/2}},$$

which yields the lower estimate in (3.18).

We next prove the upper estimate in (3.18). It is readily seen that $\exp\{-\frac{(1-u)\sqrt{xy}}{ct}\}\le 1$ and hence $A_t(\kappa;x,y)\le c'$. On the other hand, from the above it follows that

$$A_t(\kappa; x, y) \le \frac{t^\kappa}{(\sqrt{xy})^\kappa} \int_0^\infty e^{-v/c} v^{\kappa-1}\, dv = \frac{c'' t^\kappa}{(\sqrt{xy})^\kappa}.$$

Together, these two estimates yield

$$A_t(\kappa; x, y) \le \frac{c^\star t^\kappa}{(\sqrt{xy}+t)^\kappa},$$

implying

$$\prod_{i=1}^{d+1} A_t(\kappa_i; x_i, y_i) \le \frac{c^\star t^{|\kappa|}}{\prod_{i=1}^{d+1}(\sqrt{x_i y_i}+t)^{\kappa_i}}. \tag{3.19}$$

To show that this leads to the desired upper estimate, we need the following simple inequality (see [6, (7.5)]):

$$|\sqrt{x_i} - \sqrt{y_i}| \le d_{\mathbb{T}}(x, y), \qquad i = 1, \dots, d+1,\ x, y \in \mathbb{T}^d.$$

This along with (2.22) implies

$$(\sqrt{x_i} + \sqrt{t})(\sqrt{y_i} + \sqrt{t}) \le c(\sqrt{x_i y_i} + t)\left(1 + \frac{d_{\mathbb{T}}(x, y)}{\sqrt{t}}\right),$$

which leads to

$$\begin{aligned}\prod_{i=1}^{d+1}(x_i+t)^{\kappa_i/2}(y_i+t)^{\kappa_i/2} &\sim \prod_{i=1}^{d+1}(\sqrt{t}+\sqrt{x_i})^{\kappa_i}(\sqrt{t}+\sqrt{y_i})^{\kappa_i}\\ &\le c\prod_{i=1}^{d+1}(\sqrt{x_i y_i}+t)^{\kappa_i}\left(1+\frac{d_{\mathbb{T}}(x,y)}{\sqrt{t}}\right)^{|\kappa|}\\ &\le c(\varepsilon)\prod_{i=1}^{d+1}(\sqrt{x_i y_i}+t)^{\kappa_i}\exp\left\{\varepsilon|\kappa|\frac{d_{\mathbb{T}}(x,y)^2}{t}\right\}.\end{aligned}$$

Here for the last inequality we have used (2.24) with $\mu = |\kappa|$. The above coupled with (3.19) yields the upper estimate in (3.18).

We now consider the case when one or more κ_i are 0, $1 \le i \le n+1$. In this case, the kernel representation (3.6) holds in the limit. If $\kappa_i = 0$, then the integral over u_i in (3.7) is replaced by the average of point evaluations at $u_i = 1$ and $u_i = -1$. It is easy to see that all deductions that lead to (3.18) are still valid taking into account the obvious fact that (see (3.17))

$$\lim_{\kappa\to 0+} A_t(\kappa; x, y) = \lim_{\kappa\to 0+} \kappa \int_0^1 \exp\left\{-\frac{(1-u)\sqrt{xy}}{ct}\right\}(1-u)^{\kappa-1}\, du = 1.$$

This completes the proof. ∎

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