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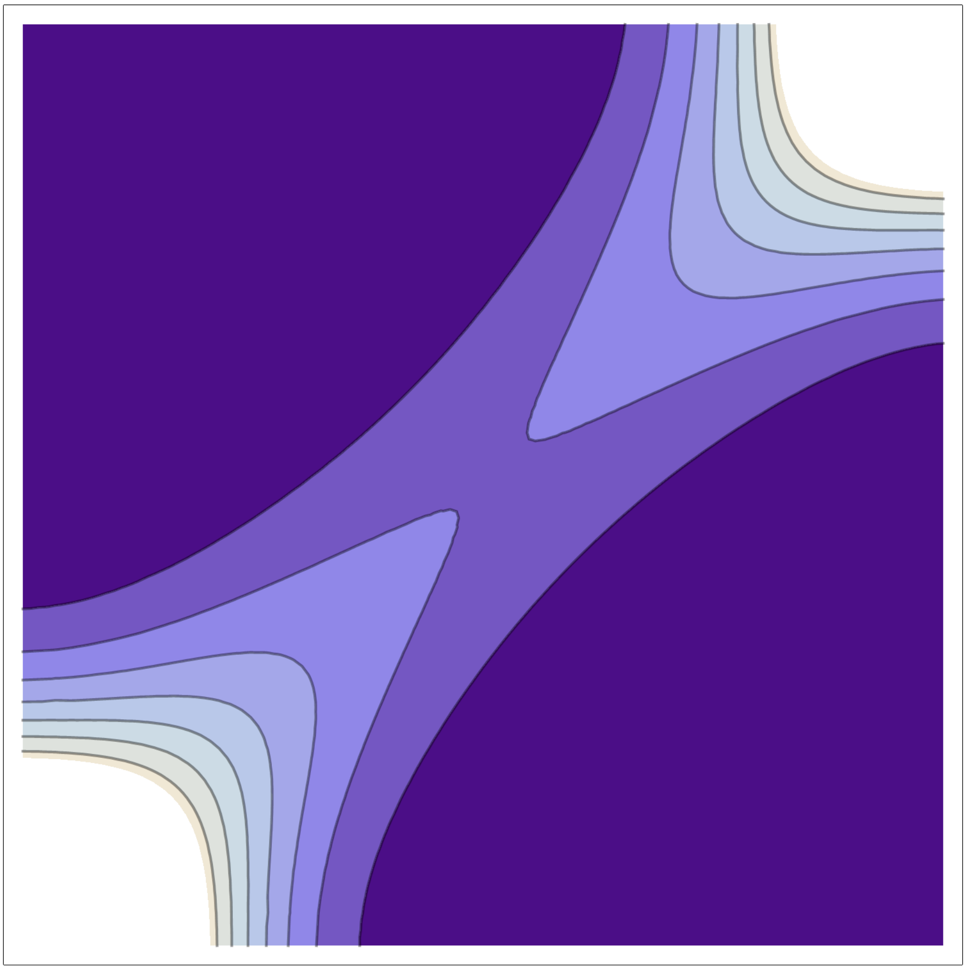

Estimates of the Spherical and Ultraspherical Heat Kernel

Master's Thesis in Engineering Mathematics and Computational Science

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Abstract

In this thesis we establish an upper bound for the spherical heat kernel on the N-dimensional unit sphere S^N for $N = 1, 2, 3$. The strategy is to use the fact that the spherical heat kernel is completely determined by the ultraspherical heat kernel. By techniques from Fourier analysis, explicit formulas for the ultraspherical heat kernel with parameter $\lambda = -1/2, 1/2$ are deduced. Also, an integral formula for the kernel with parameter $\lambda = 0$ is introduced. By estimating these formulas for the ultraspherical heat kernels, the estimates of the spherical heat kernel are obtained.

Furthermore, we prove that the periodized Gauss-Weierstrass kernel is strictly decreasing on $[0, \pi]$. Both an analytic and a probabilistic proof are given. A generalization of this result is also established for small t, saying that the spherical heat kernel on S^2 and S^3 is strictly decreasing as a function of the spherical distance between its two arguments.

Keywords: Periodized Gauss-Weierstrass kernel, spherical heat kernel, Jacobi heat kernel, ultraspherical heat kernel, Brownian motion on S^1.

Acknowledgements

I would like to express my sincere gratitude to my supervisor Peter Sjögren for the useful comments, remarks and engagement through the learning process of this master thesis. Furthermore, I would like to thank Johan Jonasson for coming up with the idea of the probabilistic proof and for helping me out with questions regarding Brownian motion and probability theory.

Daniel Andersson, Göteborg, May 20, 2013

Contents

1

Introduction

A heat kernel describes the evolution of temperature in a domain where an initial unit of heat energy is placed at one point at time $t = 0$, with the boundary conditions satisfied (if there are any). More precisely, the heat kernel is defined as the fundamental solution to the heat equation. Since the heat equation essentially is the same as the diffusion equation, the heat kernel can also be interpreted as the evolution of the probability density function for finding a diffusing particle, starting a some point at $t = 0$, in a particular area in the domain.

We will now give a more general but informal definition of the heat kernel. Let L be an appropriate elliptic operator and Ω be a domain of a manifold M equipped with a measure μ. For $t > 0$, let $p_t : \Omega \times \Omega \to \mathbb{R}$ be smooth and define the function u by

$$u(x,t) = \int_{\Omega} p_t(x,y) f(y)\, d\mu(y),$$

for a μ-integrable function f defined on Ω. Then p_t is called a *heat kernel* if u satisfies the parabolic differential equation

$$(\partial_t - L)u(x,t) = 0, \quad x, y \in \Omega, \quad t > 0,$$

with some boundary conditions, and

$$\lim_{t \to 0^+} u(x,t) = f(x).$$

That is, u satisfies the 'heat equation' and tends to the initial function f as t tends to 0.

Let us consider three examples.

1. When M and Ω are the Euclidean space $\mathbb{R}^N$ with Lebesgue measure and L is the Laplace operator, the kernel has the form

$$p_t(x,y) = \left(\frac{1}{4\pi t}\right)^{N/2} \exp\left(-\frac{d(x,y)^2}{4t}\right), \tag{1.1}$$

   where $d(x,y)$ denotes the Eulidean distance between x and y in $\mathbb{R}^N$.

2. If $M = \mathbb{R}$, $\Omega = [-1,1]$, $d\mu = (1-x^2)^{\lambda}\, dx$ (for some parameter $\lambda > -1$) and L is the ultraspherical Laplacian, we obtain the *ultraspherical heat kernel*, denoted by G_t^{λ}.

3. Let S^N denote the unit sphere in $\mathbb{R}^{N+1}$. If both M and Ω are S^N with the standard area measure and L is the Laplace-Beltrami operator, we obtain the *spherical heat kernel* denoted by K_t^N.

In contrast to (1.1), no general closed formula for K_t^N is known. However, there is a well-known upper bound given by

$$K_t^N(\xi,\eta) \leq C(\delta)\frac{1}{t^{N/2}}\exp\left(-\frac{d(\xi,\eta)^2}{4(1+\delta)t}\right), \quad \forall\delta > 0. \tag{1.2}$$

where $C(\delta)$ is a positive constant and $d(\xi,\eta)$ denotes the spherical distance between ξ and η (see [2]). Also, K_t^N is bounded from below by the same expression with $\delta = 0$.

This upper bound reminds of (1.1) except for δ. It is natural to conjecture that we can set $\delta = 0$ when the spherical distance between ξ and η is small, since $\mathbb{R}^N$ is a good approximation of the sphere in $\mathbb{R}^{N+1}$ locally. An interesting question is what happens when the spherical distance between ξ and η is large, since then the special geometry of the sphere comes into play.

It turns out that we can use the ultraspherical heat kernel to approach this problem. The spherical heat kernel is in fact completely determined by the ultraspherical heat kernel in the following way

$$G_t^\lambda\left(\cos\left[d\left(\xi,\,\eta\right)\right],1\right) \simeq K_t^N\left(\xi,\eta\right), \quad \lambda = N/2-1. \tag{1.3}$$

As a result, we obtain estimates of the spherical heat kernel by estimates of the ultrapherical heat kernel. For example, by the main result of [10] we have the following Gaussian upper bound of the ultraspherical heat kernel when $\lambda \geq -1/2$

$$G_t^\lambda\left(\cos\left[d\left(\xi,\,\eta\right)\right],1\right) \leq C\left(\frac{1}{t\left(t+\pi-\theta\right)}\right)^{\lambda+1/2}\frac{1}{\sqrt{t}}\exp\left(-c\frac{d(\xi,\,\eta)^2}{t}\right), \quad \theta\in[0,\pi], \tag{1.4}$$

where C and c are positive constants. If we could show that this formula holds true for $c = 1/4$, we obtain an estimate for the spherical heat kernel which is sharper than (1.2). The aim of this thesis is to provide such estimates for the cases $N = 1, 2$ and 3.

In addition to the estimates, we shall study the monotonicity properties of the spherical heat kernel. If an initial unit of heat energy is placed at one point on S^N at time t = 0, it is intuitively easy to accept that the temperature is lower the further away from the starting-point we get, given any time $t > 0$. Nevertheless, it turns out to be quite tricky to actually prove it. This task is the subject of Chapter 4.

Throughout the paper, we adopt the notation $X \lesssim Y$ when there exists a constant C independent of relevant parameters such that $X \leq CY$. We write $X \simeq Y$ if both $X \lesssim Y$ and $Y \lesssim X$. For a set $A \subseteq \mathbb{R}$ we denote its compliment by A^c and write $x + A := \{x + y : y \in A\}$ for $x \in A$.

2

Heat Kernels

In this chapter, we introduce the different kinds of heat kernels that we shall study. We start with the important Gauss-Weierstrass kernel and its periodization, which will be present in almost every treatment of the other kernels. Thereafter we introduce the Jacobi heat kernel of which the ultraspherical heat kernel is a special case. Then we derive explicit formulas for three of the ultraspherical heat kernels. In the final section we relate the ultraspherical heat kernel to the spherical heat kernel.

2.1 The Gauss-Weierstrass kernel and its periodization

Consider the classical heat equation on the real line:

$$\begin{cases} u_t - u_{xx} = 0, & x \in \mathbb{R}, \quad t > 0, \\ u(x,0) = g(x), & x \in \mathbb{R}. \end{cases} \tag{2.1}$$

If we assume that $g \in L^1$, we can use the Fourier transform to show that there exists a solution of the form

$$u(x,t) = W_t * g\ (x) := \int W_t(x-y) g(y)\, dy, \tag{2.2}$$

where W_t is the Gauss-Weierstrass kernel, defined by

$$W_t(x) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right), \quad x \in \mathbb{R}, \quad t > 0.$$

By analysing (2.2), one can show that the condition $g \in L^1$ can be relaxed. In fact, we have the following theorem.

Theorem 2.1. *If g is a bounded continuous function on $\mathbb{R}$, then $W_t * g(x)$ is a solution to (2.1) and $W_t * g(x)$ tends to g uniformly on every compact subset of $\mathbb{R}$ as t tends to 0. This is the unique bounded solution.*

See Theorem 8.1 and Theorem 8.8 in [7] for a proof. Let us use this result to find a solution to (2.1) in the special case when g is 2π-periodic. We have

$$\begin{aligned} u(x,t) &= \sum_{n\in\mathbb{Z}} \int_{-\pi+2\pi n}^{\pi+2\pi n} W_t(x-y)g(y)\,dy \\ &= \sum_{n\in\mathbb{Z}} \int_{-\pi}^{\pi} W_t(x-z-2\pi n)g(z)\,dz \\ &= \int_{-\pi}^{\pi} \vartheta_t(x-z)g(z)\,dz, \end{aligned} \tag{2.3}$$

where ϑ_t is the periodized Gauss-Weierstrass kernel, defined by

$$\vartheta_t(x) = \sum_{n\in\mathbb{Z}} W_t(x+2\pi n).$$

That is,

$$\vartheta_t(x) = \sum_{n\in\mathbb{Z}} \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{(x+2\pi n)^2}{4t}\right).$$

In Figure 2.1 a demonstrative graph of ϑ_t is shown.

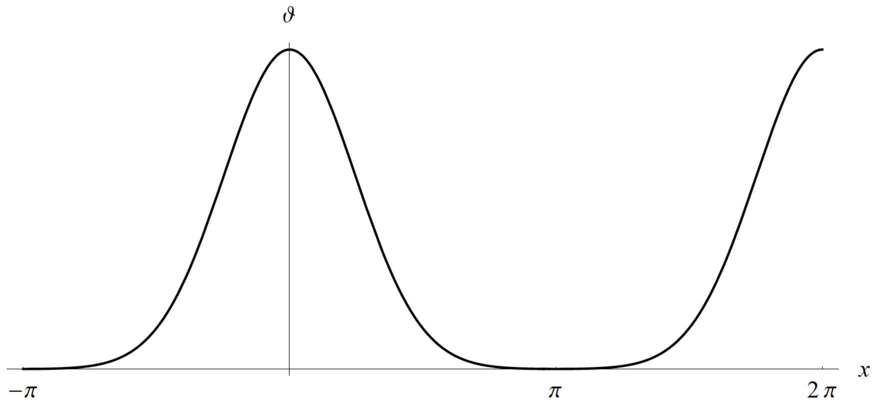

Figure 2.1: An illustration of $\vartheta_t(x)$ for $-\pi \le x \le 2\pi$ when $t = 0.3$.

It follows from the definition that ϑ_t is 2π-periodic, and we obtain an important observation if we let $g(x) = \vartheta_{t_0}(x)$ for some $t_0 > 0$. Then, according to (2.3), the solution to (2.1) is given by $\int_{-\pi}^{\pi} \vartheta_t(x-z)\vartheta_{t_0}(z)\,dz$. But it is readily seen that ϑ_{t+t_0} is also a solution to this problem and by uniquess they must be the same

$$\vartheta_{t+t_0}(x) = \int_{-\pi}^{\pi} \vartheta_t(x-z)\vartheta_{t_0}(z)\,dz. \tag{2.4}$$

This is known as the *semi-group property* of the kernel ϑ_t.

Another approach for finding a solution to (2.1) in the case when g is 2π-periodic is by using Fourier series. By the standard procedure of separation of variables one gets

$$u(x,t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} e^{-n^2 t}(a_n \cos nx + b_n \sin nx),$$

where a_n and b_n are selected to be the Fourier coefficients of g (provided that they exists). If we insert the formulas for a_n and b_n we obtain

$$u(x,t) = \frac{1}{\pi}\int_{-\pi}^{\pi}\left(\frac{1}{2} + \sum_{n=1}^{\infty} e^{-n^2 t}\cos n(x-z)\right) g(z)\,dz.$$

If we compare this with (2.3) we infer that

$$\vartheta_t(x) = \frac{1}{2\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty} e^{-n^2 t}\cos nx. \tag{2.5}$$

This result follows also directly by applying the Poisson summation formula to ϑ_t (see [4, (9.38)]). We shall use this relation later when dealing with one of the ultraspherical heat kernels. We conclude this section with some useful observations.

Observation 2.2.

1. *For all $n \in \mathbb{Z}$, the function $x \mapsto \vartheta_t(x + n\pi)$ is even.*
2. *$\vartheta_t \in C^\infty(\mathbb{R})$ and*
$$\vartheta_t^{(k)}(x) = \sum_{n\in\mathbb{Z}} W_t^{(k)}(x + 2\pi n).$$
3. *$\vartheta_t(x) + \vartheta_t(\pi - x) = 2\vartheta_{4t}(2x)$.*

Proof.

1. It suffices to show that $\vartheta_t(x)$ and $\vartheta_t(x+\pi)$ are even since ϑ_t is 2π-periodic. First we note that $\vartheta_t(x)$ can be written as
$$W_t(x) + \sum_{n\geq 1}\left[W_t(x+2\pi n) + W_t(x - 2\pi n)\right],$$
which is a sum of even functions. Similarly,
$$\vartheta_t(x+\pi) = \sum_{n\geq 0}\left[W_t(x+\pi+2\pi n) + W_t(x-\pi-2\pi n)\right],$$
which also is a sum of even functions.

2. By the Weierstrass M-test it follows that the series
$$\sum_{n\in\mathbb{Z}} W_t^{(k)}(x+2\pi n)$$
is uniformly convergent on the compact interval $[0,\pi]$ for any k. Therefore, we can interchange the differentiations and the summation.

3. If we use (2.5) together with $\cos n(\pi - x) = (-1)^n \cos nx$, we get
$$\vartheta_t(x) + \vartheta_t(\pi - x) = \frac{1}{\pi} + \frac{1}{\pi}\sum_{n=1}^{\infty}(1 + (-1)^n)e^{-n^2 t}\cos nx,$$
which implies that the terms corresponding to odd n vanish. That is,
$$\vartheta_t(x) + \vartheta_t(\pi - x) = \frac{1}{\pi} + \frac{2}{\pi}\sum_{n=1}^{\infty} e^{-4n^2 t}\cos 2nx,$$
and this is $2\vartheta_{4t}(2x)$.

□

2.2 The ultraspherical heat kernel

We will mainly be interested the ultraspherical heat kernel, which is a special case of the more general Jacobi heat kernel. Therefore, we start with stating some important properties of the Jacobi polynomials and the Jacobi heat kernel.

The Jacobi polynomials are defined by

$$P_n^{\alpha,\beta}(x) = \frac{(-1)^n}{2^n n!}(1-x)^{-\alpha}(1+x)^{-\beta}\frac{d^n}{dx^n}\left[(1-x)^{\alpha}(1+x)^{\beta}(1-x^2)^n\right],$$

for parameters $\alpha, \beta > -1$ and $n \geq 0$. They satisfies the Jacobi differential equation

$$J^{\alpha,\beta}P_n^{\alpha,\beta} = n(n+\alpha+\beta+1)P_n^{\alpha,\beta}, \tag{2.6}$$

where $J^{\alpha,\beta}$ is the Jacobi operator, given by

$$J^{\alpha,\beta} = -(1-x^2)\frac{d^2}{dx^2} - [\beta-\alpha-(\alpha+\beta+2)x]\frac{d}{dx}. \tag{2.7}$$

This means that the Jacobi polynomials are the eigenfunctions of the Jacobi operator with eigenvalues $n(n+\alpha+\beta+1)$.

For some values on the parameters α and β, other well-known polynomials are obtained. If $\alpha=\beta=0$, the Jacobi polynomials are the Legendre polynomials. For $\alpha=\beta=-1/2$, we get the Chebyshev polynomials. If $\alpha=\beta=\lambda-1/2$, they reduce to the ultraspherical polynomials C_n^{λ} up to a normalizing factor

$$P_n^{\lambda-1/2,\,\lambda-1/2}(x) = \frac{\Gamma(2\lambda)\Gamma(\lambda+n+1/2)}{\Gamma(2\lambda+n)\Gamma(\lambda+1/2)}C_n^{\lambda}(x).$$

For each α and β, the polynomials $\{P_n^{(\alpha,\beta)}\}$ form an orthogonal basis for $L^2(-1,1)$ with respect to the measure

$$d\varrho_{\alpha,\beta}(x) = (1-x)^{\alpha}(1+x)^{\beta}\,dx,$$

with the normalizing constant

$$h_n^{\alpha,\beta} := \int_{-1}^{1}\left[P_n^{\alpha,\beta}(x)\right]^2\,d\varrho_{\alpha,\beta} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)\Gamma(n+1)}. \tag{2.8}$$

Similarly to the usual series that is obtained by separation of variables when solving the heat equation, the Jacobi heat kernel is defined by

$$G_t^{\alpha,\beta}(x,y) = \sum_{n=0}^{\infty} e^{-tn(n+\alpha+\beta+1)}\frac{P_n^{\alpha,\beta}(x)P_n^{\alpha,\beta}(y)}{h_n^{\alpha,\beta}}, \quad x,y\in[-1,1], \quad t>0. \tag{2.9}$$

A difference in this kernel compared with other kernels (e.g. the Hermite and Laguerre kernel) is that the eigenvalue in the exponential is not linear in n and this difficulty is one reason why no explicit formula for $G_t^{\alpha,\beta}(x,y)$ has been found. However, for parameters $\alpha,\beta \geq -1/2$ Gaussian upper and lower bounds have been deduced (see [10]).

We shall now see that the kernel is smooth for $t>0$ and $x,y\in(-1,1)$. First we note that the k:th derivative of $P_n^{\alpha,\beta}$ can be estimated by repeated use of the formula

$$\frac{d}{dx}P_n^{\alpha,\beta}(x) = \frac{1}{2}(n+\alpha+\beta+1)P_{n-1}^{\alpha+1,\beta+1}(x),$$

(see [13, (4.21.7)]) combined with the following upper bound for Jacobi polynomials (see [13, (7.32.2)]),

$$\max_{-1\leq x\leq 1}|P_n^{\alpha,\beta}(x)|\lesssim n^q,\quad q=\max\left(\alpha,\beta,-\frac{1}{2}\right).$$

This means, the k:th derivative of $P_n^{\alpha,\beta}(x)$ is bounded by a polynomial of n having a degree depending only on α, β and k. Next, by applying the asymptotic formula

$$\lim_{n\to\infty}\frac{\Gamma(n+\alpha)}{\Gamma(n)n^\alpha}=1,\quad \alpha\in\mathbb{R},$$

to (2.8) we infer that $1/h_n^{\alpha,\beta}\lesssim n$. Thus, by differentiating the terms in the defining series by any order in x, y or t we see that the series is uniformly convergent on every compact subset of $(0,\infty)\times[-1,1]$ by Weierstrass M-test, and the derivatives can therefore be moved out in front of the summation.

The smoothness together with (2.6) implies in particular that $(\partial_t+J^{\alpha,\beta})G_t^{\alpha,\beta}(\cdot\,,y)=0$ for all $y\in[-1,1]$. In view of this we let the function U be defined by

$$U(x,t)=\int_{-1}^{1}G_t^{\alpha,\beta}(x,y)F(y)\,d\varrho_{\alpha,\beta}(y),\tag{2.10}$$

where F is a $\varrho_{\alpha,\beta}$-integrable function. Then $(\partial_t+J^{\alpha,\beta})U=0$ and furthermore, by [9, Proposition 3.3], we have $\lim_{t\to 0}U(x,t)=F(x)$. That is, U is the solution the Jacobi heat equation:

$$\begin{cases}(\partial_t+J^{\alpha,\beta})U(x,t)=0, & x\in[-1,1],\quad t>0,\\ U(x,0^+)=F(x), & x\in[-1,1].\end{cases}\tag{2.11}$$

When the Jacobi parameters are equal, $\alpha=\beta=\lambda$, the Jacobi heat kernel is called the ultraspherical heat kernel. Since this will be the case for the rest of this paper, we adopt the following notation

$$G_t^\lambda:=G_t^{\lambda,\lambda},\quad J^\lambda:=J^{\lambda,\lambda},\quad h_n^\lambda=h_n^{\lambda,\lambda},\quad \varrho_\lambda:=\varrho_{\lambda,\lambda}.$$

Furthermore, we shall use the trigonometric parametrization $x=\cos\theta$, which transforms the operator J^λ into the new operator

$$\mathcal{J}^\lambda=-\frac{d^2}{d\theta^2}-\frac{(2\lambda+1)\cos\theta}{\sin\theta}\frac{d}{d\theta},\tag{2.12}$$

and the measure transforms to

$$d\varrho_\lambda(\cos\theta)=2\sin^{2\lambda+1}\theta\,d\theta.$$

For more properties of the Jacobi and ultraspherical polynomials, see chapter 4 in [13].

As mentioned earlier, there is no closed formula for G_t^λ in general. But for the special cases $\lambda=-1/2$ and $1/2$, the kernels can be expressed as 'nice' non-oscillating series, and when $\lambda=0$ the kernel can be expressed as an integral with a positive non-oscillating integrand. In each of the next three subsections these cases will studied separately.

2.2.1 Neumann boundary conditions

We shall now use the classical heat equation on $[0, \pi]$ with Neumann boundary conditions to establish that

$$G_t^{-1/2}(\cos\theta,\, \cos\varphi) = \vartheta_t(\theta-\varphi) + \vartheta_t(\theta+\varphi), \quad \theta,\varphi \in [0,\pi], \quad t>0. \tag{2.13}$$

We start by noting that if $\lambda = -1/2$, the differential operator (2.12) turns out to be particularity simple, $\mathcal{J}^{-1/2} = -\partial_{\theta\theta}$, and the measure $\varrho_{-1/2}$ becomes simply the Lebesgue measure in θ. If we set $u(\theta,t) := U(\cos\theta, t)$ and $f(\varphi) := F(\cos\varphi)$, the problem (2.11) transforms into

$$\begin{cases} (\partial_t - \partial_{\theta\theta})u(\theta,t) = 0, & \theta \in [0,\pi], \quad t>0 \\ u(\theta,0) = f(\theta), & \theta \in [0,\pi], \end{cases}$$

and the solution is thus given by

$$u(\theta,t) = \int_0^\pi G_t^{-1/2}(\cos\theta,\, \cos\varphi) f(\varphi)\, d\varphi. \tag{2.14}$$

If follows that u satisfies the Neumann boundary condition $u_\theta(0,t) = u_\theta(\pi,t) = 0$ since $G_t^{-1/2}$ is smooth and

$$u_\theta(\theta,t) = \sin\theta \int_0^\pi (\partial_x G_t^{-1/2})(\cos\theta, \cos\varphi) f(\varphi)\, d\varphi. \tag{2.15}$$

Hence u is a solution to the classical heat problem with Neumann boundary conditions:

$$\begin{cases} u_t - u_{\theta\theta} = 0, & \theta \in [0,\pi], \quad t>0, \\ u(\theta,0) = f(\theta), & \theta \in [0,\pi], \\ u_\theta(0,t) = u_\theta(\pi,t) = 0, & t>0. \end{cases} \tag{2.16}$$

By using the maximum principle, one can show that the solution to (2.16) is unique. See section 2 in [11].

Next, we use a different approach to find another solution to (2.16). Then we compare the two solutions obtained and conclude that the two corresponding kernels must be equal.

Let g be the even 2π-periodic extension of f. That is,

$$g(\theta) = \begin{cases} f(\theta - 2n\pi) & \text{if } \theta \in [2n\pi,\, 2n\pi+\pi] \\ f(2n\pi - \theta) & \text{if } \theta \in [2n\pi - \pi,\, 2n\pi], \end{cases} \qquad \forall n \in \mathbb{Z}.$$

In this way, $\theta \mapsto g(n\pi + \theta)$ is an even function for all $n \in \mathbb{Z}$. From Section 2.1 we know that $W_t * g(x)$ is a solution to (2.1). Let us define the function u to be the restriction of $W_t * g(x)$ on $[0,\pi]$. Then, u will be a solution to (2.16) if also the boundary condition $u_\theta(0,t) = u_\theta(\pi,t) = 0$ is satisfied. This is indeed the case, because

$$u_\theta(0,t) = \int W_t'(-\phi) g(\phi)\, d\phi = 0,$$

since W_t' is odd and g is even. Similarly,

$$u_\theta(\pi,t) = \int W_t'(-\phi') g(\pi + \phi')\, d\phi' = 0,$$

since W_t' is odd and $\theta \mapsto g(\pi+\theta)$ is even. Thus the boundary conditions are satisfied and u is a solution to (2.16).

To derive the corresponding heat kernel, we write

$$\begin{aligned} u(\theta,t) &= \sum_{n\in\mathbb{Z}} \left(\int_{2n\pi}^{2n\pi+\pi} W_t(\theta-\phi) f(\phi-2n\pi)\,d\phi + \int_{2n\pi-\pi}^{2n\pi} W_t(\theta-\phi) f(2n\pi-\phi)\,d\phi \right) \\ &= \sum_{n\in\mathbb{Z}} \left(\int_0^{\pi} W_t(\theta-\varphi-2n\pi) f(\varphi)\,d\varphi + \int_0^{\pi} W_t(\theta+\varphi-2n\pi) f(\varphi)\,d\varphi \right), \end{aligned}$$

and by the dominated convergence theorem we can interchange the sum and integral to get

$$\begin{aligned} u(\theta,t) &= \int_0^{\pi} \sum_{n\in\mathbb{Z}} \left[W_t(\theta-\varphi-2n\pi) + W_t(\theta+\varphi-2n\pi)\right] f(\varphi)\,d\varphi \\ &= \int_0^{\pi} \left[\vartheta_t(\theta-\varphi) + \vartheta_t(\theta+\varphi)\right] f(\varphi)\,d\varphi. \end{aligned} \tag{2.17}$$

So the kernel is given by $\vartheta_t(\theta-\varphi)+\vartheta_t(\theta+\varphi)$. Since (2.14) and (2.17) both solve the problem (2.16), the two kernels must be the same and we conclude that (2.13) is true.

2.2.2 Dirichlet boundary conditions

Now we use the same technique as in the previous subsection, but with Neumann replaced by Dirichlet boundary conditions. The aim is to show that

$$G_t^{1/2}(\cos\theta,\,\cos\varphi) = e^t\,\frac{\vartheta_t(\theta-\varphi)-\vartheta_t(\theta+\varphi)}{\sin\theta\sin\varphi}, \quad \theta,\varphi\in[0,\pi], \quad t>0. \tag{2.18}$$

When $\lambda = 1/2$, the differential operator (2.12) will not be as simple as before. Instead, we get

$$\mathcal{J}^{1/2} = -\frac{d^2}{d\theta^2} - \frac{2\cos\theta}{\sin\theta}\frac{d}{d\theta}, \tag{2.19}$$

and the measure (2.2) is

$$d\varrho_{1/2}(\cos\theta) = 4\sin^2\theta\,d\theta. \tag{2.20}$$

Therefore, we consider the new basis functions ϕ_n defined by

$$\phi_n(\theta) = 2\sin\theta P_n^{1/2}(\cos\theta), \tag{2.21}$$

which then form a complete orthogonal basis for $L^2(0,\pi)$ with respect to Lebsegue measure in θ. Furthermore, according to (2.6) we have

$$\mathcal{J}^{1/2}P_n^{1/2}(\cos\theta) = n(n+2)P_n^{1/2}(\cos\theta), \tag{2.22}$$

from which it follows directly that

$$\sin\theta\mathcal{J}^{1/2}\left[\frac{1}{\sin\theta}\phi_n(\theta)\right] = n(n+2)\phi_n(\theta). \tag{2.23}$$

If we expand the LHS according to (2.19) we get

$$\sin\theta\left(-\frac{1}{\sin\theta}\phi_n''(\theta) - \left[2\left(\frac{1}{\sin\theta}\right)' + \frac{2\cos\theta}{\sin^2\theta}\right]\phi_n'(\theta) + \left[\frac{2\cos^2\theta}{\sin^3\theta} - \left(\frac{1}{\sin\theta}\right)''\right]\phi_n(\theta)\right), \tag{2.24}$$

which simply reduces to $-\phi_n''(\theta) - \phi_n(\theta)$ when expanding the square brackets. This implies that (2.23) is equivalent to

$$-\phi_n''(\theta) = (n+1)^2\phi_n(\theta). \tag{2.25}$$

Thus we can use ϕ_n to solve the classical heat problem with Dirichlet boundary conditions:

$$\begin{cases} u_t - u_{xx} = 0, & x \in [0,\pi], \quad t > 0, \\ u(x,0) = f(x), & x \in [0,\pi], \\ u(0,t) = u(\pi,t) = 0, & t > 0. \end{cases} \tag{2.26}$$

This problem has a unique solution by the maximum principle (see [7, Theorem 8.7]). By the standard procedure of separation of variables, we get the solution

$$u(\theta,t) = \int_0^\pi \sum_{n=0}^\infty e^{-t(n+1)^2}\frac{\phi_n(\theta)\phi_n(\varphi)}{\|\phi_n\|^2}f(\varphi)\,d\varphi,$$

where $\|\cdot\|$ is the norm in $L^2(0,\pi)$. It is readily seen from (2.21) that u satisfies the boundary conditions

$$u(0,t) = u(\pi,t) = 0.$$

By inspecting the kernel we note from (2.9) that it can be written as

$$\begin{aligned} \sum_{n=0}^\infty e^{-t(n+1)^2}\frac{\phi_n(\theta)\phi_n(\varphi)}{\|\phi_n\|^2} &= \sum_{n=0}^\infty e^{-tn(n+2)}\frac{P_n^{1/2}(\cos\theta)P_n^{1/2}(\sin\varphi)}{\|P^{1/2}\|_\varrho^2}e^{-t}\sin\theta\sin\phi \\ &= G_t^{1/2}(\cos\theta,\cos\varphi)e^{-t}\sin\theta\sin\phi. \end{aligned} \tag{2.27}$$

In the same manner as in the previous section, we shall find another solution to (2.26) and thereafter conclude that the corresponding heat kernel must be equal to (2.27) by uniqueness. This time, we let g be the *odd* 2π-periodic extension of f. That is,

$$g(\theta) = \begin{cases} f(\theta - 2n\pi) & \text{if } \theta \in [2n\pi,\, 2n\pi+\pi] \\ -f(2n\pi - \theta) & \text{if } \theta \in [2n\pi - \pi,\, 2n\pi]. \end{cases} \qquad \forall n \in \mathbb{Z}.$$

In this way, $\theta \mapsto g(n\pi + \theta)$ is an odd function for all $n \in \mathbb{Z}$. Let the function u be the restriction of $W_t * g$ on $[0,\pi]$. Then u will be a solution to (2.26) if also the boundary condition $u(0,t) = u(\pi,\, t) = 0$ is satisfied. This is indeed the case, because

$$u(0,t) = \int W_t(-\phi)g(\phi)\,d\phi = 0,$$

since W_t is even and g is odd. Similarly,

$$u(\pi,t) = \int W_t(-\phi')g(\pi+\phi')\,d\phi' = 0,$$

since W_t is even and $\theta \mapsto g(\pi+\theta)$ is odd. Thus u is a solution to (2.26).

To derive the corresponding heat kernel, we note that

$$\begin{aligned} u(\theta,t) &= \int W_t(\theta-\varphi)g(\varphi)\,d\varphi \\ &= \sum_{n\in\mathbb{Z}}\left(\int_{2n\pi}^{2n\pi+\pi} W_t(\theta-\varphi)f(\varphi-2n\pi)\,d\varphi - \int_{2n\pi-\pi}^{2n\pi} W_t(\theta-\varphi)f(2n\pi-\varphi)\,d\varphi\right), \end{aligned}$$

which is exactly the same expression obtained in the previous subsection except for a minus sign instead of a plus sign. By carrying out exactly the same calculations we get the solution

$$u(\theta,t) = \int_0^\pi [\vartheta_t(\theta-\varphi) - \vartheta_t(\theta+\varphi)]\, f(\varphi)\, d\varphi.$$

So the kernel is given by $\vartheta_t(\theta-\varphi) - \vartheta_t(\theta+\varphi)$ and has to be equal to (2.27),

$$G_t^{1/2}(\cos\theta, \cos\varphi) e^{-t} \sin\theta \sin\phi = \vartheta_t(\theta-\varphi) - \vartheta_t(\theta+\varphi),$$

so (2.18) is true as desired.

2.2.3 The Dirichlet-Mehler integral

In the two previous subsections we have found elementary representations of the kernels $G_t^{-1/2}$ and $G_t^{1/2}$ in terms of ϑ_t. Unfortunately, it is not possible to use the same technique to derive a similar result for G_t^0. However, there exists a double integral representation of G_t^0 in terms of $G_t^{1/2}$ as a result of the more general formula discovered by the authors of [10] (Theorem 3.1),

$$G_t^{\alpha,\beta}(\cos\theta,\, \cos\varphi) = C_{\alpha,\beta} \iint G_{t/4}^{\alpha+\beta+1/2}\left(u \sin\frac{\theta}{2}\sin\frac{\varphi}{2} + v\cos\frac{\theta}{2}\cos\frac{\varphi}{2}, 1\right) d\Pi_\alpha(u)\, d\Pi_\beta(v), \tag{2.28}$$

where Π_α is the measure defined on the interval $[-1,1]$ by

$$d\Pi_\alpha(u) = \frac{\Gamma(\alpha+1)}{\sqrt{\pi}\Gamma(\alpha+1/2)}(1-u^2)^{\alpha-1/2}\, du,$$

and $C_{\alpha,\beta} = \sqrt{\pi}\Gamma(\alpha+\beta+3/2)/\left(2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)\right)$. The proof relies on Dijksma and Koornwinder's product formula for Jacobi polynomials which in turn is a result of sophisticated mathematics (see [3]).

The remainder of this section is intended to give an alternative proof of (2.28) for the case we shall be mainly interested in; $\varphi = \alpha = \beta = 0$. The key observation is that the Jacobi polynomials reduces to Legendre polynomials in this setting and the strategy is to insert the Dirichlet-Mehler's integral formula for the Legendre polynomials into the oscillatory sum (2.9) defining G_t^0.

The Dirichlet-Mehler integral formula for Legendre polynomials P_n is given by

$$P_n(\cos\theta) = \frac{2}{\pi}\int_\theta^\pi \frac{\sin(n+\frac{1}{2})\phi}{\sqrt{2\cos\theta - 2\cos\phi}}\, d\phi,$$

and can be proved by using Cauchy's integral formula on Rodrigues' formula for P_n, with a cleverly selected contour of integration. See [13, (4.8.7)] for proof and details. We shall modify this formula slightly to make the interval of integration symmetric around $\pi/2$, which is crucial for the later argument. To do this, note that the interval of integration can be extended to $[\theta, 2\pi-\theta]$ since the integrand is "even around $\phi = \pi$",

$$\frac{1}{\pi}\int_\theta^{2\pi-\theta} \frac{\sin(n+\frac{1}{2})\phi}{\sqrt{2\cos\theta - 2\cos\phi}}\, d\phi.$$

Next, the transformation $\gamma = \phi/2$ yields the desired expression

$$P_n(\cos\theta) = \frac{2}{\pi}\int_{\theta/2}^{\pi-\theta/2} \frac{\sin(2n+1)\gamma}{\sqrt{2\cos\theta - 2\cos 2\gamma}}\, d\gamma. \tag{2.29}$$

We now establish an integral formula for $G_t^0(\cos\theta,\,1)$, which later will be the starting point when estimating the spherical heat kernel on S^2.

Theorem 2.3. *Let $t>0$ and $\theta\in[0,\pi]$. Then*

$$G_t^0(\cos\theta,1)=e^{t/4}\int_{\theta/2}^{\pi-\theta/2}\frac{-\vartheta'_{t/4}(\gamma)}{\sqrt{2\cos\theta-2\cos 2\gamma}}\,d\gamma. \tag{2.30}$$

Proof. Let us simply denote P_n^0 by P_n and let $\|\cdot\|$ be the norm in $L^2(-1,1)$. From (2.9) we have

$$G_t^0(\cos\theta,1)=\sum_{n=0}^{\infty}e^{-tn(n+1)}\frac{P_n(\cos\theta)P_n(1)}{\|P_n\|^2}. \tag{2.31}$$

By induction on Bonnet's recursion formula

$$(n+1)P_{n+1}(x)=(2n+1)xP_n(x)-nP_{n-1}(x),\quad P_0(x)=1,\quad P_1(x)=x,$$

we can prove that $P_n(1)=1$ for all n (see [12, 12.2]). From (2.8) it follows that $\|P_n\|^2=2/(2n+1)$ (or see Theorem 6.1 in [4]). If we insert the formula (2.29) into (2.31) and write $n(n+1)=\frac14(2n+1)^2-\frac14$ we get

$$G_t^0(\cos\theta,1)=\frac{e^{t/4}}{\pi}\sum_{n=0}^{\infty}\int_{\theta/2}^{\pi-\theta/2}e^{-\frac{t}{4}(2n+1)^2}(2n+1)\sin(2n+1)\gamma\frac{1}{\sqrt{2\cos\theta-2\cos 2\gamma}}\,d\gamma.$$

The expression in the square root is symmetric around $\gamma=\pi/2$ and the integral of $\sin n\gamma$ over the interval $[\theta/2,\,\pi-\theta/2]$ vanishes whenever n is even. Hence we can sum over all $n\geq 0$ and get

$$\frac{e^{t/4}}{\pi}\sum_{n=1}^{\infty}\int_{\theta/2}^{\pi-\theta/2}e^{-\frac{t}{4}n^2}n\sin n\gamma\frac{1}{\sqrt{2\cos\theta-2\cos 2\gamma}}\,d\gamma.$$

By the dominated convergence theorem we move the summation inside the integral,

$$e^{t/4}\int_{\theta/2}^{\pi-\theta/2}\left[\frac{1}{\pi}\sum_{n=1}^{\infty}e^{-\frac{t}{4}n^2}n\sin n\gamma\right]\frac{1}{\sqrt{2\cos\theta-2\cos 2\gamma}}\,d\gamma.$$

Then we recognize the expression in square brackets as the derivative of the periodized Gauss-Weierstrass kernel,

$$\frac{1}{\pi}\sum_{n=1}^{\infty}e^{-\frac{t}{4}n^2}n\sin n\gamma=-\frac{d}{d\gamma}\left(\frac{1}{2\pi}+\frac{1}{\pi}\sum_{n=1}^{\infty}e^{-\frac{t}{4}n^2}\cos n\gamma\right)=-\vartheta'_{t/4}(\gamma),$$

by (2.5). This proves the assertion. □

We shall now show that (2.30) can be transformed into the general formula (2.28) as a special case. In view of (2.18) we obtain

$$G_t^{1/2}(\cos\gamma,1)=\lim_{\varphi\to 0}\frac{2e^t}{\sin\gamma}\left(-\frac{\vartheta_t(\gamma+\varphi)-\vartheta_t(\gamma-\varphi)}{2\sin\varphi}\right)=\frac{2e^t}{\sin\gamma}\left(-\vartheta'_t(\gamma)\right). \tag{2.32}$$

Using this together with the trigonometric identity $\cos(2a) - \cos(2b) = 2\left(\cos^2 a - \cos^2 b\right)$, the integral formula (2.30) can be written as

$$G_t^0(\cos\theta, 1) = \frac{1}{4}\int_{\theta/2}^{\pi-\theta/2} G_{t/4}^{1/2}\big(\cos\gamma, 1\big)\frac{\sin\gamma}{\sqrt{\cos^2\frac{\theta}{2} - \cos^2\gamma}}\, d\gamma.$$

The transformation

$$v = \frac{\cos\gamma}{\cos\frac{\theta}{2}}, \quad dv = -\frac{\sin\gamma}{\cos\frac{\theta}{2}}d\gamma,$$

yields

$$G_t^0(\cos\theta, 1) = \frac{1}{4}\int_{-1}^{1} G_{t/4}^{1/2}\left(v\cos\frac{\theta}{2}, 1\right)\frac{1}{\sqrt{1-v^2}}\, dv, \tag{2.33}$$

which indeed is the special case of (2.28) when $\varphi = \alpha = \beta = 0$. We shall use this formula later when proving that the function $\theta \mapsto G_t^0(\cos\theta, 1)$ is decreasing on $[0, \pi]$ for small t.

2.3 The spherical heat kernel

The Laplace operator can be generalized to arbitrary Riemannian manifolds and goes then usually by the name of Laplace-Beltrami operator. Let $f \in C^2(S^N)$ and $F : \mathbb{R}^{N+1}\backslash\{0\} \to \mathbb{R}$ be defined by $F(x) = f(x/|x|)$. Then the corresponding Laplace-Beltrami operator, denoted Δ_N, on the sphere can be defined by $\Delta_N f := \Delta F|_{S^N}$, that is, the ordinary Laplacian in $\mathbb{R}^{N+1}$ applied to F and restricted to S^N (see [1, p. 15]).

The heat equation on the sphere is

$$\begin{cases} u_t - \Delta_N u = 0, & x \in S^N, \quad t > 0 \\ u(x,\, 0^+) = f(x), & x \in S^N. \end{cases} \tag{2.34}$$

Let σ_N be the standard non-normalized area measure on S^N. Then the solution of (2.34) is given by

$$u(\xi, t) = \int_{S^N} K_t^N(\xi, \eta) f(\eta)\, d\sigma_N(\eta),$$

where K_t^N is expressed as an oscillatory series of spherical harmonics.

By properties of the Laplacian, the kernel K_t^N depends only on ξ and η through their spherical distance, which is defined by

$$d(\xi, \eta) = \arccos\langle \xi, \eta\rangle.$$

To see this, recall that the ordinary Laplacian in $\mathbb{R}^{N+1}$ satisfies $\Delta(f \circ U) = (\Delta f) \circ U$ for functions $f \in C^2(\mathbb{R}^N)$ and orthogonal linear transformations U. By the way we defined Δ_N, it is clear that also $\Delta_N(f \circ U) = (\Delta_N f) \circ U$ for $f \in C^2(S^N)$. This implies in particular that $(\partial_t - \Delta_N)K_t^N(U\xi, U\eta) = 0$ with respect to ξ for all η. Furthermore, since the measure σ_N is invariant under orthogonal transformations and $u(x, 0^+) = f(x)$, we also have

$$\begin{aligned} \lim_{t\to 0}\int_{S^N} K_t^N(U\xi, U\eta) f(\eta)\, d\sigma_N(\eta) &= \lim_{t\to 0}\int_{S^N} K_t^N(U\xi, \eta') f(U^{-1}\eta')\, d\sigma_N(\eta') \\ &= f(U^{-1}\eta')|_{\eta' = U\xi} = f(\xi). \end{aligned}$$

This means that the function $(\xi, \eta) \mapsto K_t^N(U\xi,\, U\eta)$ also is a kernel of the problem (2.34), and therefore we must have

$$K_t^N(\xi,\, \eta) = K_t^N(U\xi,\, U\eta), \tag{2.35}$$

by uniqueness. For any points $\xi_1, \eta_1, \xi_2, \eta_2$ in S^N such that $d(\xi_1, \eta_1) = d(\xi_2,\, \eta_2)$, there exists an orthogonal transformation U such that $\xi_1 = U\xi_2$ and $\eta_1 = U\eta_2$. By (2.35) we then have $K_t^N(\xi_1,\, \eta_1) = K_t^N(\xi_2,\, \eta_2)$, which means that the spherical heat kernel only depends on the spherical distance between its arguments. For this reason, it is convenient to adopt the following notation

$$K_t^N(\theta) := K_t^N(\xi,\, \eta), \quad \theta = d(\xi, \eta).$$

By Theorem 3.3 in [10] we have the following relation between the spherical and ultraspherical heat kernel

$$G_t^\lambda(x,\, y) = \int_{S^{N-1}} K_t^N\left((x, \xi_2, \ldots, \xi_N),\, \left(y, \zeta\sqrt{1-y^2}\right)\right) d\sigma_{N-1}(\zeta), \quad x, y \in [-1, 1], \quad t > 0,$$

where the coordinates $\xi_2, \ldots, \xi_N$ can be picked arbitrarily and $\lambda = N/2 - 1$. By letting $y = 1$, we see that the variable of integration vanishes from the integrand and we infer that

$$G_t^\lambda(x, 1) = \sigma_{N-1}\left(S^{N-1}\right) K_t^N\left((x, \xi_2, \ldots, \xi_N),\, (1, 0, \ldots,\, 0)\right). \tag{2.36}$$

The constant $\sigma_{N-1}\left(S^{N-1}\right)$ is the 'area' of S^{N-1} and is given by $2\pi^{N/2}/\Gamma(N/2)$ (see [14, p. 193-194]). Let $x = \cos\theta$ and note that the spherical distance between $(x, \xi_2, \ldots, \xi_N)$ and $(1, 0, \ldots,\, 0)$ is θ. By the notation introduced earlier, we can write (2.36) as

$$K_t^N(\theta) = \frac{\Gamma(\lambda+1)}{2\pi^{\lambda+1}} G_t^\lambda(\cos\theta, 1), \quad \lambda = \frac{N}{2} - 1.$$

In view of the expressions for $G_t^\lambda(\cos\theta, 1)$ with parameter $\lambda = -1/2$, 0 and $1/2$ we derived earlier, we have the following theorem.

Theorem 2.4. *For $t > 0$ and $\theta \in [0, \pi]$, we have*

$$\begin{aligned}
K_t^1(\theta) &= \vartheta_t(\theta), \\
K_t^2(\theta) &= \frac{e^{t/4}}{2\pi} \int_{\theta/2}^{\pi-\theta/2} \frac{-\vartheta'_{t/4}(\gamma)}{\sqrt{2\cos\theta - 2\cos 2\gamma}}\, d\gamma, \\
K_t^3(\theta) &= \frac{e^t}{2\pi}\left(\frac{-\vartheta'_t(\theta)}{\sin\theta}\right).
\end{aligned}$$

Proof. This follows from (2.13), (2.30) and (2.32), respectively. □

See Figure 4.1 for an illustration of $K_t^3(\theta)$ for $t = 0.4$ and $0 \le \theta \le \pi$. The formulas in Theorem 2.4 will be the starting-point of the estimates of K_t^1, K_t^2 and K_t^3.

3

Preparatory results

In the expressions for K_t^2 and K_t^3 in Theorem 2.4, the derivative of ϑ_t is present. The function ϑ_t' behaves very much like W_t' for small t, which is convenient since W_t' is an elementary function and easy to handle. But at the right endpoint we have $\vartheta_t'(\pi) = 0$ (by Observation 2.2) in contrast to $W_t'(\pi) < 0$, for all t. This detail will later be important and makes it insufficient to approximate ϑ_t' by just W_t'. It turns out to be useful to introduce the auxiliary function $h_t = \vartheta_t'/W_t'$, and in this way access the behavior of ϑ_t' near π in terms of h_t and W_t'.

3.1 Properties of the auxiliary function

Definition 3.1. *For $t > 0$ we define $h_t(x)$ by*

$$h_t(x) = \frac{\vartheta_t'(x)}{W_t'(x)}, \quad 0 < x \leq \pi,$$

and as $\lim_{x\to 0^+} h_t(x)$ *at* $x = 0$.

In Figure 3.1 a typical graph of h_t is demonstrated.

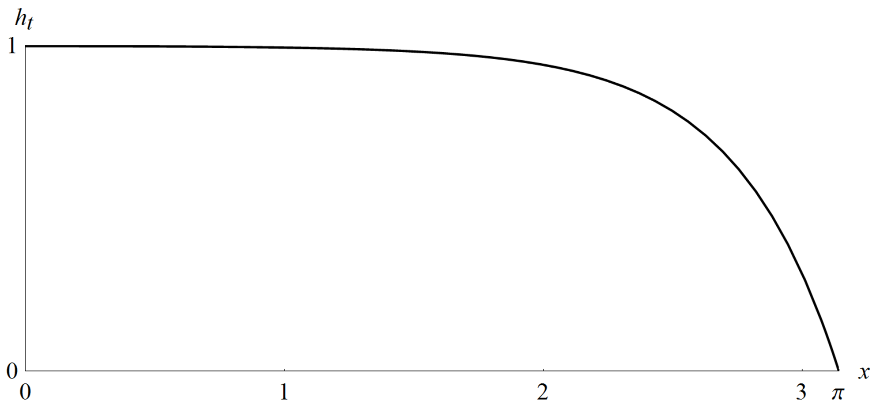

Figure 3.1: An illustration of $h_t(x)$ for $t = 1$ and $0 \leq x \leq \pi$.

We shall prove that h_t is strictly concave and then use this to show that h_t is strictly decreasing. Since $\vartheta_t'(\pi) = 0$ we also have $h_t(\pi) = 0$, which then implies that h_t is non-negative on $[0,\pi]$. From these properties we obtain a useful upper bound for h_t, which we will use later in the estimates of the spherical heat kernels. But first we shall verify that h_t can be written as

$$h_t(x) = 1 + \sum_{n\geq 1} f_{n,t}(x) \exp\left(-\frac{\pi^2 n^2}{t}\right) \tag{3.1}$$

where

$$f_{n,t}(x) := 2\cosh\left(\frac{\pi n x}{t}\right) - \frac{4\pi n}{x}\sinh\left(\frac{\pi n x}{t}\right).$$

This expression is useful since we then can use $f_{n,t}$ to prove properties of h_t. The formula (3.1) follows from the following calculations

$$\begin{aligned} h_t(x) &= \sum_{n\in\mathbb{Z}} \left(1+\frac{2\pi n}{x}\right)\exp\left(-\frac{\pi^2 n^2 + \pi n x}{t}\right) \\ &= 1 + \sum_{n\geq 1}\left[\left(1+\frac{2\pi n}{x}\right)\exp\left(-\frac{\pi n x}{t}\right) + \left(1-\frac{2\pi n}{x}\right)\exp\left(\frac{\pi n x}{t}\right)\right]\exp\left(-\frac{\pi^2 n^2}{t}\right) \\ &= 1 + \sum_{n\geq 1}\left[2\cosh\left(\frac{\pi n x}{t}\right) - \frac{4\pi n}{x}\sinh\left(\frac{\pi n x}{t}\right)\right]\exp\left(-\frac{\pi^2 n^2}{t}\right). \end{aligned}$$

Theorem 3.2. *h_t is strictly concave on $[0,\pi]$ when t is small.*

Proof. In view of (3.1), the idea is to show that the second derivative of $f_{n,t}$ is negative for $n \geq 1$ when t is sufficiently small. Then it follows that h_t is strictly concave for small t. We have

$$\frac{d^2 f_{n,t}}{dx^2}(x) = \left(\frac{2\pi^2 n^2}{t^2} + \frac{8\pi^2 n^2}{x^2 t}\right)\cosh\left(\frac{n\pi x}{t}\right) - \left(\frac{8\pi n}{x^3} + \frac{4\pi^3 n^3}{x t^2}\right)\sinh\left(\frac{n\pi x}{t}\right).$$

Let us assume that $x \in (0,\pi]$. Then by multiplying both sides with $\frac{t^3 x^3}{2n\pi}$, we get

$$\frac{d^2 f_{n,t}}{dx^2}(x) < 0 \Leftrightarrow \left(n\pi x^3 t + 4n\pi t^2 x\right)\cosh\left(\frac{n\pi x}{t}\right) - \left(4t^3 + 2n^2\pi^2 x^2 t\right)\sinh\left(\frac{n\pi x}{t}\right) < 0. \tag{3.2}$$

Let us denote the LHS of the last inequality by $F_{n,t}(x)$ and observe that $F_{n,t}(0) = 0$. Then (3.2) is true (except at $x = 0$) if $F_{n,t}$ is strictly decreasing on $(0,\pi]$ for all $n \geq 1$ when t is sufficiently small. Indeed, if we take the derivative of $F_{n,t}$ and use the inequality $\sinh < \cosh$, we obtain

$$\begin{aligned} F'_{n,t}(x) &= \left(3n\pi x^2 t - 2n^3\pi^3 x^2\right)\cosh\left(\frac{n\pi x}{t}\right) + n^2\pi^2 x^3 \sinh\left(\frac{n\pi x}{t}\right) \\ &< n\pi x^2\left(3t - n\pi(2n\pi - x)\right)\cosh\left(\frac{n\pi x}{t}\right) \\ &< 0, \quad n \geq 1, \quad x \in (0,\pi], \quad 0 < t < \frac{\pi^2}{3}. \end{aligned}$$

Hence $F'_{n,t}$ is negative and $F_{n,t}$ is strictly decreasing, implying that (3.2) is true for $x \in (0,\pi]$ and we are done. □

Corollary 3.3. *h_t is strictly decreasing on $[0,\pi]$ for small t.*

Proof. We note that h_t is the quotient of two odd functions and is therefore even. Thus we have $h_t'(0) = 0$. This fact, together with Theorem 3.2 proves the assertion. $\square$

Theorem 3.4. *For sufficiently small t we have the following upper bound*

$$h_t(x) \leq \min\left(1, \frac{\pi}{t}(\pi - x)\right), \quad x \in [0, \pi].$$

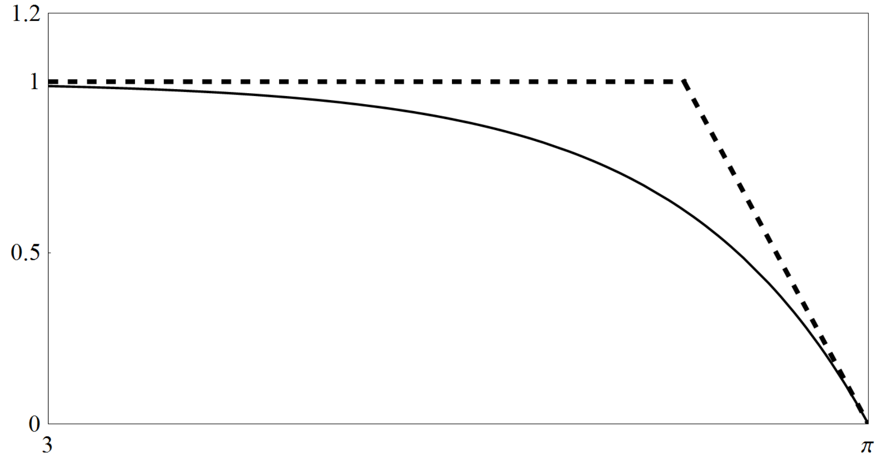

Figure 3.2: An illustration of Theorem 3.4 for $x \in [3, \pi]$ with $t = 0.1$. The solid line is h_t and the dashed line is the upper bound.

Proof of Theorem 3.4. Let us first prove that $h_t(x) \leq 1$ for $x \in [0, \pi]$ and then prove that $h_t(x) \leq \frac{\pi}{t}(\pi - x)$ for $x \in [0, \pi]$.

It was proved in Corollary 3.3 that h_t is strictly decreasing. If we can show that $h_t(0) < 1$ for sufficiently small t, the first inequality follows. Indeed, recall from (3.1) that

$$h_t(x) = 1 + \sum_{n \geq 1} f_{n,t}(x) \exp\left(-\frac{\pi^2 n^2}{t}\right)$$

and note that

$$f_{n,t}(0) = 2 - \frac{4\pi^2 n^2}{t} < 0, \quad n \geq 1, \quad t < 2\pi^2.$$

Hence $h_t(x) \leq 1$ for $x \in [0, \pi]$ for small t.

Now we show that $h_t(x) \leq \frac{\pi}{t}(\pi - x)$ for $x \in [0, \pi]$. From Theorem 3.2 we also know that h_t is strictly concave on $[0, \pi]$. The idea is therefore to find an upper bound for the tangent line of h_t at $x = \pi$. Looking at the derivative of h_t, we get

$$\begin{aligned} h_t'(\pi) &= \sum_{n \geq 1} f_{n,t}'(\pi) \exp\left(-\frac{\pi^2 n^2}{t}\right) \\ &= \sum_{n \geq 1} \left[\left(\frac{2\pi n}{t} + \frac{4n}{\pi}\right) \sinh\left(\frac{\pi^2 n}{t}\right) - \frac{4\pi n^2}{t} \cosh\left(\frac{\pi^2 n}{t}\right)\right] \exp\left(-\frac{\pi^2 n^2}{t}\right). \end{aligned}$$

The first term in this series tends to $-\infty$ as t gets small:

$$\left[\left(\frac{2\pi}{t} + \frac{4}{\pi}\right) \sinh\left(\frac{\pi^2}{t}\right) - \frac{4\pi}{t} \cosh\left(\frac{\pi^2}{t}\right)\right] \exp\left(-\frac{\pi^2}{t}\right) = -\frac{\pi}{t} + \frac{2}{\pi} - \left(\frac{3\pi}{t} + \frac{2}{\pi}\right) \exp\left(-\frac{2\pi^2}{t}\right).$$

We shall now verify that sum of the remaining terms tends to 0 as $t \to 0$. By using the triangle inequality and the fact that $\sinh < \cosh < \exp$ we get

$$\begin{aligned}\sum_{n\geq 2} |f'_{n,t}(\pi)| \exp\left(-\frac{\pi^2 n^2}{t}\right) &\leq \sum_{n\geq 2}\left(\frac{2\pi n}{t} + \frac{4n}{\pi} + \frac{4\pi n^2}{t}\right)\exp\left(\frac{\pi^2(n-n^2)}{t}\right) \\ &\lesssim \frac{1}{t}\sum_{n=1}^{\infty} n^2 \exp\left(-\frac{\pi^2 n}{t}\right),\end{aligned}$$

and this well-known series can be evaluated to

$$\frac{e^{\frac{-\pi^2}{t}}\left(1+e^{\frac{-\pi^2}{t}}\right)}{t\left(1-e^{\frac{-\pi^2}{t}}\right)^3},$$

(see [12, p. 192]) which indeed tends to 0 as $t \to 0$. The analysis just made shows that we have

$$h'_t(\pi) = -\frac{\pi}{t} + \frac{2}{\pi} + O\left(\frac{1}{t}\exp\left(-\frac{\pi^2}{t}\right)\right),$$

and thus,

$$h'_t(\pi) \geq -\frac{\pi}{t},$$

for sufficiently small t. Hence $h_t(x) \leq \frac{\pi}{t}(\pi - x)$ on $[0, \pi]$ and we are done. $\square$

Corollary 3.5. *For $x \in [0, \pi]$ and sufficiently small t we have the following bound*

$$h_t(x) \lesssim \frac{\pi - x}{\pi - x + t}.$$

Proof. By Theorem 3.4 it suffices to show that

$$G_t(x) := (\pi + 1)\frac{\pi - x}{\pi - x + t} - \min\left(1, \frac{\pi}{t}(\pi - x)\right) \geq 0.$$

Observe that we have equality at $x = \pi - t/\pi$ and $x = \pi$. It is easy to verify that G_t is concave on the two intervals $[0,\, \pi - t/\pi]$ and $[\pi - t/\pi,\, \pi]$. By this it follows directly that $G_t(x) \geq 0$ on the latter interval. If we pick t sufficiently small such that $G_t(0) > 0$ we get that $G_t(x) \geq 0$ on the first interval as well. $\square$

It should be noted that the arguments in this sections only apply when t is small, but it is natural to conjecture that similar results hold for all t.

4

Monotonicity properties of the spherical heat kernel

In this chapter, we show that $K_t^N(\theta)$ is strictly decreasing on $[0,\pi]$ when $N = 1$, 2 and 3. That is, the spherical heat kernel $K_t^N(\xi,\eta)$ is strictly decreasing as a function of the spherical distance between ξ and η. By the methods used, we shall only consider small t for $N = 2, 3$. Also, a probabilistic proof is given for the case when $N = 1$. In view of Theorem 2.4, this implies in particular that the kernels are positive.

4.1 Monotonicity of K_t^1

The idea is to show that the derivative of ϑ_t is negative on $(0,\pi)$ for sufficiently small t and then use the semi-group property of ϑ_t to prove that ϑ_t remains strictly decreasing on $[0,\pi]$ for all t. But first we need the following elementary lemma.

Lemma 4.1. *Let f and g be 2π-periodic functions which are integrable on $[0,2\pi]$. Then,*

$$\int_{-\pi}^{\pi} f(x-y)g(y)\,dy = \int_{-\pi}^{\pi} g(x-y)f(y)\,dy, \quad x \in [0,\pi].$$

Proof. By the change of variables, $z = x - y$, the LHS becomes

$$\begin{aligned}
\int_{x-\pi}^{x+\pi} f(z)g(x-z)\,dz &= \int_{x-\pi}^{\pi} f(z)g(x-z)\,dz + \int_{\pi}^{x+\pi} f(z)g(x-z)\,dz \\
&= \int_{x-\pi}^{\pi} f(z)g(x-z)\,dz + \int_{-\pi}^{x-\pi} f(z)g(x-z)\,dz \\
&= \int_{-\pi}^{\pi} g(x-z)f(z)\,dz.
\end{aligned}$$

□

Theorem 4.2. *ϑ_t is strictly decreasing on $[2\pi n, 2\pi n+\pi]$ and strictly increasing on $[2\pi n+\pi, 2\pi n+2\pi]$ for all $n \in \mathbb{Z}$, $t > 0$.*

Proof. Since $\vartheta_t(x)$ and $\vartheta_t(x+\pi)$ is even and 2π-periodic, it suffices to show that ϑ_t is strictly decreasing on $[0,\pi]$ for all $t>0$.

If we use the relation $\vartheta_t' = h_t W_t'$, and recall that h_t is positive and W_t' is negative on $(0,\pi)$, we conclude that ϑ_t is strictly decreasing on $[0,\pi]$ for small t. Accordingly, let $t_0>0$ be sufficiently small so that ϑ_{t_0} is strictly decreasing on $[0,\pi]$, and let $t\in(0,t_0]$. From (2.4) we know that ϑ_t satisfies the semi-group property

$$\vartheta_{t_0+t}(x) = \int_{-\pi}^{\pi} \vartheta_{t_0}(x-z)\vartheta_t(z)\,dz.$$

Differentiating both sides and using Lemma 4.1, we obtain

$$\vartheta_{t_0+t}'(x) = \int_{-\pi}^{\pi} \vartheta_t(x-z)\vartheta_{t_0}'(z)\,dz.$$

Since ϑ_{t_0}' is odd, we have

$$\vartheta_{t_0+t}'(x) = \int_0^{\pi} \left[\vartheta_t(x-y) - \vartheta_t(x+y)\right]\vartheta_{t_0}'(y)\,dy. \tag{4.1}$$

It turns out that the expression in the square brackets is positive:

$$\vartheta_t(x-y) - \vartheta_t(x+y) > 0, \quad x,y\in(0,\pi). \tag{4.2}$$

To verify this, observe first that

$$\vartheta_t(x) = \vartheta_t(\arccos(\cos x)), \quad x\in\mathbb{R},$$

since both ϑ_t and cos are 2π-periodic and even, and $\arccos\cos x = x$ when $x\in[0,\pi]$. With this observation and the fact that ϑ_t and arccos are strictly decreasing on $[0,\pi]$ and $[-1,1]$ respectively, we get the following equivalences

$$\begin{aligned}
\vartheta_t(z-y) - \vartheta_t(z+y) > 0 \quad &\Leftrightarrow \quad \vartheta_t(\arccos(\cos(x-y))) - \vartheta_t(\arccos(\cos(x+y))) > 0\\
&\Leftrightarrow \quad \arccos(\cos(x-y)) - \arccos(\cos(x+y)) < 0\\
&\Leftrightarrow \quad \cos(x-y) - \cos(x+y) > 0\\
&\Leftrightarrow \quad 2\sin x\sin y > 0.
\end{aligned}$$

Thus (4.2) is true.

Hence the RHS of (4.1) is negative for $x\in(0,\pi)$, which implies that ϑ_{t_0+t} is strictly decreasing on $[0,\pi]$. Since this is true for all $t\in(0,t_0]$ we infer that ϑ_t is strictly decreasing on $[0,\pi]$ for all $t<2t_0$. We can now iterate the whole procedure to show that ϑ_t is strictly decreasing on $[0,\pi]$ for $t<2^k t_0$ for any $k\in\mathbb{N}$. Hence ϑ_t is decreasing on $[0,\pi]$ for all $t>0$. □

Corollary 4.3. *ϑ_t has a global maximum at $z=2\pi n$ and global minimum at $2\pi n+\pi$ for $n\in\mathbb{Z}$.*

4.2 Monotonicity of K_t^3

Theorem 4.4. *$K_t^3(\theta)$ is strictly decreasing on $[0,\pi]$ when t is sufficiently small.*

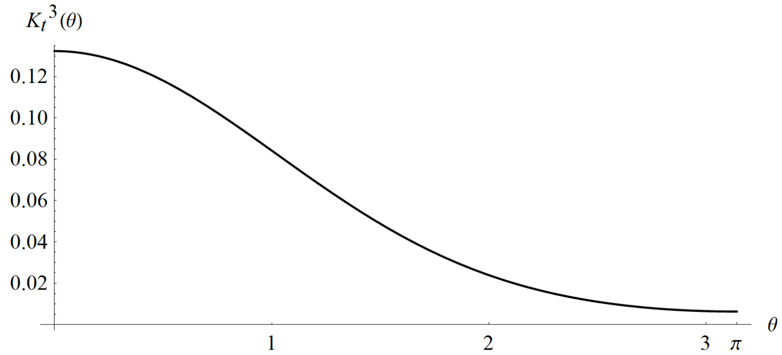

Figure 4.1: An illustration of $K_t^3(\theta)$ for $t = 0.4$ and $0 \leq \theta \leq \pi$.

Proof of Theorem 4.4. Recall from Theorem 2.4 that

$$K_t^3(\theta) = \frac{e^t}{2\pi}\left(-\frac{\vartheta_t'(\theta)}{\sin\theta}\right).$$

Our strategy is to show that the derivative is negative for $\theta \in (0, \pi)$,

$$\frac{d}{d\theta}\left(-\frac{\vartheta_t'(\theta)}{\sin\theta}\right) < 0 \Leftrightarrow -\frac{\vartheta_t''(\theta)}{\sin\theta} + \frac{\vartheta_t'(\theta)}{\sin^2\theta}\cos\theta < 0,$$

which is equivalent to showing that

$$\vartheta_t''(\theta)\sin\theta - \vartheta_t'(\theta)\cos\theta > 0 \tag{4.3}$$

for $\theta \in [0, \pi]$. To prove this, we consider two cases; when θ is small and large, respectively.

Case 1: Assume that $\theta \in [0, \pi/2]$. If we now use the relation $\vartheta_t' = h_t W_t'$, the inequality (4.3) becomes

$$h_t'(\theta)W_t'(\theta)\sin\theta + h_t(\theta)\left[W_t''(\theta)\sin\theta - W_t'(\theta)\cos\theta\right] > 0.$$

To get rid of the derivatives of W_t we use the fact that

$$W_t'(\theta) = -\frac{\theta}{2t}W_t(\theta),$$

to get

$$-h_t'(\theta)\frac{\theta\sin\theta}{2t}W_t(\theta) + h_t(\theta)\left[\left(\frac{\theta^2}{4t^2} - \frac{1}{2t}\right)\sin\theta + \frac{\theta}{2t}\cos\theta\right]W_t(\theta) > 0. \tag{4.4}$$

Since h_t is strictly decreasing for small t by Corollary 3.3, the first term is positive on the whole interval $(0, \pi)$. For the second term, note first that the expression in square brackets is zero at $\theta = 0$, and that its derivative is given by

$$\frac{\theta^2\cos\theta}{4t^2} + (1-t)\frac{\theta\sin\theta}{2t^2} \tag{4.5}$$

which clearly is positive for $\theta \in (0, \pi/2)$ when $t < 1$. This implies that the second term is positive on $(0, \pi/2)$. Thus, (4.3) is true for $\theta \in (0, \pi/2)$ when t is small.

Case 2: Assume that $\theta \in [\pi/2, \pi]$. Note that the function $\theta \mapsto \vartheta_t''(\theta)\sin\theta - \vartheta_t'(\theta)\cos\theta$ is zero at $\theta = \pi$. If we can show that its derivative is negative on $[\pi/2, \pi]$ we are done. The derivative is given by

$$\frac{d}{d\theta}\left[\vartheta_t''(\theta)\sin\theta - \vartheta_t'(\theta)\cos\theta\right] = \left(\vartheta_t^{(3)}(\theta) + \vartheta_t'(\theta)\right)\sin\theta.$$

From Theorem 4.2 we know that ϑ_t' is negative on $[\pi/2, \pi]$. Thus it remains to prove that $\vartheta_t^{(3)}$ is negative on $[\pi/2, \pi]$ for small t.

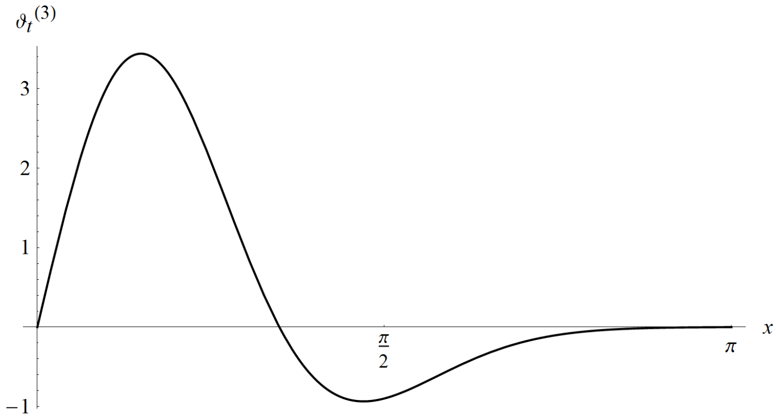

Figure 4.2: $\vartheta_t^{(3)}$ for $t = 0.2$ and $0 \leq x \leq \pi$. The critical points will move to the left as t gets small.

Observe that this holds true for the Gauss-Weierstrass kernel:

$$W_t^{(3)}(\theta) = \left(\frac{3\theta}{4t^2} - \frac{\theta^3}{8t^3}\right) W_t(\theta), \tag{4.6}$$

which indeed is negative when $\sqrt{6t} < \theta$. From the defining formula of ϑ_t we have

$$\begin{aligned}\vartheta_t^{(3)}(\theta) &= \sum_{n\in\mathbb{Z}} W_t^{(3)}(\theta + 2\pi n) \\ &= \sum_{n\geq 0}\left(W_t^{(3)}(\theta + 2\pi n) + W_t^{(3)}(\theta - 2\pi(n+1))\right).\end{aligned}$$

If we can show that all the terms in this series are non-positive when t is small we are done. Let t be so small that $W_t^{(3)}(\theta + 2\pi n)$ is negative. Then

$$W_t^{(3)}(\theta + 2\pi n) + W_t^{(3)}(\theta - 2\pi(n+1)) \leq 0 \quad \Leftrightarrow \quad \frac{-W_t^{(3)}(\theta - 2\pi(n+1))}{W_t^{(3)}(\theta + 2\pi n)} \leq 1.$$

If we use (4.6) and move the exponential term over to the RHS we get

$$\frac{(2\pi n + 2\pi - \theta)^3 - 6(2\pi n + 2\pi - \theta)t}{(2\pi n + \theta)^3 - 6(2\pi n + \theta)t} \leq \exp\left(\frac{\pi(2n+1)(\pi - \theta)}{t}\right), \quad \theta \in [\pi/2,\, \pi], \quad n \geq 0.$$

For every fixed $\theta \in [\pi/2, \pi]$ and t sufficiently small, the LHS is decreasing and the RHS is increasing as functions of n. This is readily seen to be true for the RHS, but for the LHS we need a few lines of argument. Let $x_n = 2\pi n + \theta$ and $y = 2\pi - 2\theta$. Then the LHS can be rewritten as

$$1 + \frac{y^3 - 6ty}{x_n^3 - 6tx_n} + 3y\frac{x_n + y}{x_n^2 - 6t},$$

and it is clear that the first two terms are nonincreasing as n is increasing provided t is small. It remains to verify that the same holds for the last term. We have

$$\begin{aligned}
\frac{x_{n+1} + y}{x_{n+1}^2 - 6t} < \frac{x_n + y}{x_n^2 - 6t} \quad &\Leftrightarrow \quad \frac{2\pi + x_n + y}{(4\pi^2 + 4\pi x_n) + x_n^2 - 6t} < \frac{x_n + y}{x_n^2 - 6t} \\
&\Leftrightarrow \quad 2\pi(x_n^2 - 6t) < (4\pi^2 + 4\pi x_n)(x_n + y) \\
&\Leftrightarrow \quad 0 < 2\pi x_n^2 + 4\pi^2(x_n + y) + 4\pi x_n y + 12\pi t,
\end{aligned}$$

which clearly is true since all terms are positive. Hence it suffices to just consider the case when $n = 0$,

$$\frac{(2\pi - \theta)^3 - 6(2\pi - \theta)t}{\theta^3 - 6\theta t} \leq \exp\left(\frac{\pi(\pi - \theta)}{t}\right), \quad \theta \in [\pi/2, \pi].$$

Note first that we have equality at $\theta = \pi$. Let $\epsilon > 0$ be sufficiently small. By differentiating the LHS with respect to θ, we obtain a continuous function which is bounded on the compact interval $(t, \theta) \in [0, \epsilon] \times [\pi/2, \pi]$ by a positive constant M. This means that the LHS is bounded above by the function $y(\theta) := -M(\theta - \pi) + 1$ on $[\pi/2, \pi]$ when $0 < t < \epsilon$. The RHS is convex function of θ and its derivative tends to $-\infty$ uniformly as t gets small, which implies that it is bounded from below by $y(\theta)$ on $[\pi/2, \pi]$ for sufficiently small t. This proves the inequality. $\square$

4.3 Monotonicity of K_t^2

Theorem 4.5. *$K_t^2(\theta)$ is strictly decreasing on $[0, \pi]$ for small t.*

Proof. From (2.33) we have

$$K_t^2(\theta) = \frac{1}{8\pi}\int_{-1}^{1} G_{t/4}^{1/2}\left(v\cos\frac{\theta}{2}, 1\right)\frac{1}{\sqrt{1 - v^2}}\,dv.$$

Let us set $f(v, \theta) = \arccos\left(v\cos\frac{\theta}{2}\right)$ for $v \in [-1, 1]$ and $\theta \in [0, \pi]$ so that $\cos f(u, \theta) = v\cos\frac{\theta}{2}$. We can then also write $G_{t/4}^{1/2}\left(v\cos\frac{\theta}{2}, 1\right)$ as $K_{t/4}^3(f)$. Note that the partial derivative

$$f_\theta'(v, \theta) = \frac{v\sin\frac{\theta}{2}}{2\sin f(v,\theta)}$$

is an odd function of v for all $\theta \in [0, \pi]$ because $f(-v, \theta) = \pi - f(v, \theta)$. By the chain rule, the derivative of the integrand is

$$\frac{d}{d\theta}\left[K_{t/4}^3(f)\frac{1}{\sqrt{1 - v^2}}\right] = \frac{d}{df}\left[K_{t/4}^3(f)\right]\frac{f_\theta'(v, \theta)}{\sqrt{1 - v^2}}.$$

Since the kernel $K_{t/4}^3$ is smooth, and $f_\theta'(v, \theta)$ is bounded and continuous with respect to v when $\theta \in (0, \pi)$, we can differentiate the integral and move the derivative inside the integral by dominated convergence. That is,

$$\frac{d}{d\theta}\left[K_t^2(\theta)\right] = \frac{1}{8\pi}\int_{-1}^{1}\frac{d}{df}\left[K_{t/4}^3(f)\right]\frac{f_\theta'(v, \theta)}{\sqrt{1 - v^2}}\,dv.$$

Since $f'_\theta(v,\theta)$ is odd, this can be written as

$$\frac{1}{8\pi}\int_0^1 \frac{d}{df}\left[K^3_{t/4}(f) - K^3_{t/4}(\pi - f)\right]\frac{f'_\theta(v,\theta)}{\sqrt{1-v^2}}\,dv.$$

By Theorem 4.4 we know that the function $K^3_{t/4}$ is strictly decreasing on $[0,\pi]$ for small t, and therefore it is clear that the square bracket is a decreasing function on $[0,\pi]$ with respect to f, which implies that the derivative is negative. Thus the integral is negative and the claim follows. □

4.4 A probabilistic proof

In this section we establish that ϑ_t is strictly decreasing on $[0,\pi]$ by using a probabilistic argument. Let Θ_t be a Brownian motion in $\mathbb{R}$ starting at 0. Then the projection of Θ_t on $S^1 = \mathbb{R}/2\pi\mathbb{Z}$ describes a freely diffusing particle on S^1. Let $\theta_1, \theta_2 \in [0,\pi]$ be such that $\theta_2 > \theta_1$. Let $\epsilon > 0$ be small and set

$$I_1 = \bigcup_{n\in\mathbb{Z}} [\theta_1 - \epsilon, \theta_1 + \epsilon] + 2\pi n, \quad \text{and} \quad I_2 = \bigcup_{n\in\mathbb{Z}} [\theta_2 - \epsilon, \theta_2 + \epsilon] + 2\pi n.$$

The probability of finding Θ_t in the set I_1 can then be interpreted as the probability of finding the diffusing particle in the interval $[\theta_1 - \epsilon, \theta_1 + \epsilon]$ on S^1 and similarly for I_2. See Figure 4.3.

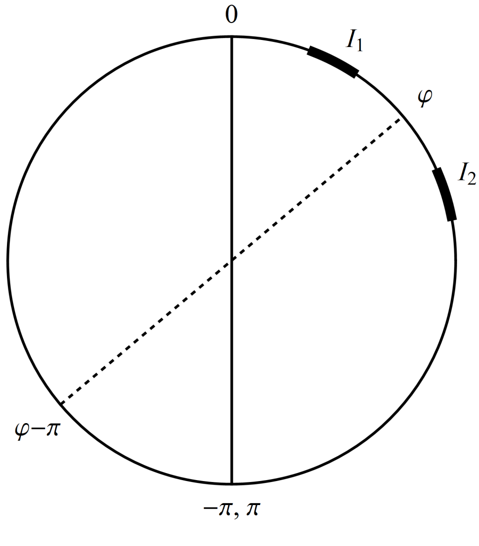

Figure 4.3: The diffusing particle will start at 0 when $t = 0$ and we wish to show that at any time $t > 0$ there is a strictly higher probability of finding it in I_1 than I_2.

For the sake of clarity, we break up the argument into a sequence of steps.

1. Relate the probabilities of finding the particle in I_1 and I_2 to ϑ_t.

2. Show that the probability of finding the particle in I_1 is greater or equal to the probability of finding it in I_2 and use this to prove that ϑ_t is nonincreasing on $[0,\pi]$.

3. Show that if the particle has crossed the dashed line in Figure 4.3 before time t, then the probability of finding it in I_1 is the same as that of finding it in I_2.

4. Establish that there is a non-zero probability of finding the particle in I_1 without ever crossing the dashed line and use this to prove that ϑ_t is strictly decreasing on $[0, \pi]$.

Step 1. Since Θ_t is a Brownian motion, it has normal distribution with mean 0 and variance t. That is, for Borel sets I of $\mathbb{R}$ we have

$$\mathbb{P}(\Theta_t \in I) = \int_I W_{t/2}(\theta)\, d\theta. \tag{4.7}$$

The probability of finding the particle in I_1 will then be

$$\begin{aligned} \mathbb{P}(\Theta_t \in I_1) &= \sum_{n\in\mathbb{Z}} \int_{[\theta_1-\epsilon,\, \theta_1+\epsilon]+2\pi n} W_{t/2}(\theta)\, d\theta \\ &= \sum_{n\in\mathbb{Z}} \int_{[\theta_1-\epsilon,\, \theta_1+\epsilon]} W_{t/2}(\theta + 2\pi n)\, d\theta \\ &= \int_{[\theta_1-\epsilon,\, \theta_1+\epsilon]} \vartheta_{t/2}(\theta)\, d\theta. \end{aligned} \tag{4.8}$$

Similarly for I_2,

$$\mathbb{P}(\Theta_t \in I_2) = \int_{[\theta_2-\epsilon,\, \theta_2+\epsilon]} \vartheta_{t/2}(\theta)\, d\theta. \tag{4.9}$$

This means that $\vartheta_{t/2}$ can be interpreted as the distribution obtained by wrapping the normal distribution around the unit circle.

Step 2. Let $\varphi = (\theta_2 + \theta_1)/2$ be the midpoint between the intervals I_1, I_2 and let τ be the stopping time defined by

$$\tau = \inf\{t > 0 : \Theta_t \in (\varphi - \pi, \varphi)^c\}. \tag{4.10}$$

Then $\{t \geq \tau\}$ represents the event that the particle has crossed the dashed line in Figure 4.3. It is proved in [6, Theorem 3.13] that stopping times defined like τ are almost surely finite; $\mathbb{P}(\tau < \infty) = 1$.

Next we use τ to write

$$\mathbb{P}(\Theta_t \in I_1) = \mathbb{P}(\Theta_t \in I_1, t \geq \tau) + \mathbb{P}(\Theta_t \in I_1,\ t < \tau), \tag{4.11}$$

and similarly

$$\mathbb{P}(\Theta_t \in I_2) = \mathbb{P}(\Theta_t \in I_2, t \geq \tau) + \underbrace{\mathbb{P}(\Theta_t \in I_2,\ t < \tau)}_{=0}. \tag{4.12}$$

The second term vanishes since Brownian motion is continuous and cannot reach I_2 without first reaching φ or $\pi - \varphi$. Let us for the moment assume that

$$\mathbb{P}(\Theta_t \in I_1, t \geq \tau) = \mathbb{P}(\Theta_t \in I_2, t \geq \tau). \tag{4.13}$$

Then, subtracting (4.12) from (4.11) implies that

$$\mathbb{P}(\Theta_t \in I_1) - \mathbb{P}(\Theta_t \in I_2) = \mathbb{P}(\Theta_t \in I_1, t < \tau) \geq 0. \tag{4.14}$$

In view of (4.8) and (4.9) and the above inequality, we obtain

$$\lim_{\epsilon\to 0} \frac{\mathbb{P}(\Theta_t \in I_1) - \mathbb{P}(\Theta_t \in I_2)}{2\epsilon} = \vartheta_{t/2}(\theta_1) - \vartheta_{t/2}(\theta_2) \geq 0.$$

Thus we conclude that ϑ_t is nonincreasing on $[0, \pi]$.

Step 3. Now we prove that (4.13) is true. By the law of total probability we have

$$\mathbb{P}(\Theta_t \in I_1, t \geq \tau) = \mathbb{P}(\Theta_t \in I_1, t \geq \tau, \Theta_\tau = \varphi) + \mathbb{P}(\Theta_t \in I_1, t \geq \tau, \Theta_\tau = \varphi - \pi),$$

and

$$\mathbb{P}(\Theta_t \in I_2, t \geq \tau) = \mathbb{P}(\Theta_t \in I_2, t \geq \tau, \Theta_\tau = \varphi) + \mathbb{P}(\Theta_t \in I_2, t \geq \tau, \Theta_\tau = \varphi - \pi).$$

Let us show that the terms corresponding to $\Theta_\tau = \varphi$ are equal. Showing that the terms corresponding to $\Theta_\tau = \varphi - \pi$ are equal can be done completely analogously.

Assume that $\mathbb{P}(t \geq \tau, \Theta_\tau = \varphi) > 0$ since otherwise we are trivially done. Then it suffices to show that

$$\mathbb{P}(\Theta_t \in I_1 \mid t \geq \tau, \Theta_\tau = \varphi) = \mathbb{P}(\Theta_t \in I_2 \mid t \geq \tau, \Theta_\tau = \varphi).$$

To prove this we need to recall the strong Markov property for Brownian motion (see for example [6]).

Theorem 4.6 (Strong Markov Property)**.** *Let τ be a almost surely finite stopping time relative to the filtration $\{\mathcal{F}_t\}$ of the standard Brownian motion $\{B_t : t \geq 0\}$. For $s \geq 0$, define the new process*

$$B_s^* = B_{s+\tau} - B_\tau$$

with filtration $\{\mathcal{F}_s^*\}$. Then $\{B_s^* : s \geq 0\}$ is a standard Brownian motion and $\mathcal{F}_s^*$ is independent of $\mathcal{F}_\tau$ for all $s > 0$.

This means that the new Brownian motion B_s^* is independent of τ and "everything we know" about B_t up to time τ. We can invoke the strong Markov property by writing $\{\Theta_t \in I_1\} = \{\Theta_{t-\tau+\tau} - \Theta_\tau \in I_1 - \Theta_\tau\} = \{\Theta_{t-\tau}^* \in I_1 - \Theta_\tau\}$ and thus

$$\begin{aligned} \mathbb{P}(\Theta_t \in I_1 \mid t \geq \tau, \Theta_\tau = \varphi) &= \mathbb{P}\left(\Theta_{t-\tau}^* \in I_1 - \Theta_\tau \mid t \geq \tau, \Theta_\tau = \varphi\right) \\ &= \mathbb{P}\left(\Theta_{t-\tau}^* \in I_1 - \varphi \mid t \geq \tau\right). \end{aligned}$$

Let $F(x) = \mathbb{P}(\tau \leq x \mid \tau \leq t)$. Since $\{\Theta_s^* : s \geq 0\}$ is independent of τ, we can marginalize over τ to obtain

$$\mathbb{P}\left(\Theta_{t-\tau}^* \in I_1 - \varphi \mid t \geq \tau\right) = \int_0^t \mathbb{P}\left(\Theta_{t-x}^* \in I_1 - \varphi\right) dF(x).$$

Similarly for I_2 we obtain

$$\mathbb{P}(\Theta_t \in I_2 \mid t \geq \tau, \Theta_\tau = \varphi) = \int_0^t \mathbb{P}\left(\Theta_{t-x}^* \in I_2 - \varphi\right) dF(x).$$

By (4.7) we see that for any interval I and $s \geq 0$ we have $\mathbb{P}(\Theta_s^* \in I) = \mathbb{P}(\Theta_s^* \in -I)$ since $W_{s/2}$ is even. But it is easy to verify that $I_1 - \varphi = -(I_2 - \varphi)$ and then we infer that the two integrands are equal. Hence (4.13) is true.

Step 4. So far we have proved that ϑ_t is nonincreasing on $[0, \pi]$. To show that it is strictly decreasing, we need some further arguments.

Let us assume there exists an open interval J in $[0, \pi]$ on which ϑ_t is constant and show that this leads to a contradiction. Since the two intervals I_1 and I_2 in our setting are arbitrary, we may assume that they are contained in J. Then, since ϑ_t is constant on J we immediately get $\mathbb{P}(\Theta_t \in I_1) = \mathbb{P}(\Theta_t \in I_2)$ by (4.7), and in view of (4.14) this implies that

$$\mathbb{P}(\Theta_t \in I_1, t < \tau) = 0. \tag{4.15}$$

We shall now show that this is false. Let σ be the stopping time defined by $\sigma = \inf\{t > 0 : \Theta_t \in (-\theta_1, \theta_1)^c\}$. The idea is to show that given $\Theta_\sigma = \theta_1$, there is a positive probability of the particle to remain in the interval $[\theta_1 - \epsilon, \theta_1 + \epsilon]$ all the time from σ up to t.

It is easy to verify that the probability $p := \mathbb{P}(\sigma < t)$ is positive for any t since $\{\Theta_{t/2} \geq \theta_1\} \subseteq \{t \geq \sigma\}$ and $\mathbb{P}(\Theta_{t/2} \geq \theta_1) = \int_{\theta_1}^{\infty} W_{t/4}\, d\theta > 0$. By symmetry the event $\{\sigma < t, \Theta_\sigma = \theta_1\}$ has probability $p/2$ and is therefore also positive. By conditioning on this event we get

$$\mathbb{P}\left(\Theta_t \in I_1, t < \tau\right) \geq \mathbb{P}\left(\Theta_t \in I_1, t < \tau \mid \sigma < t, \Theta_\sigma = \theta_1\right) p/2.$$

By using the strong Markov property we can write $\{\Theta_t \in I_1\} = \{\Theta_{t-\sigma+\sigma} - \Theta_\sigma \in I_1 - \Theta_\sigma\} = \{\widetilde{\Theta}^*_{t-\sigma} \in I_1 - \Theta_\sigma\}$ where $\widetilde{\Theta}^*_s := \Theta_{s+\sigma} - \Theta_\sigma$, is the new Brownian motion, independent of σ and $\{\Theta_t : t \leq \sigma\}$, starting at $t = \sigma$. Then the conditional probability can be written as

$$\begin{aligned}
\mathbb{P}\left(\widetilde{\Theta}^*_{t-\sigma} \in I_1 - \Theta_\sigma, t < \tau \mid \sigma < t,\ \Theta_\sigma = \theta_1\right) &= \mathbb{P}\left(\widetilde{\Theta}^*_{t-\sigma} \in [-\epsilon,\, \epsilon], t < \tau \mid \sigma < t\right) \\
&\geq \mathbb{P}\left(\sup_{s\in[0,\, t-\sigma]} \left|\widetilde{\Theta}^*_s\right| < \epsilon \mid \sigma < t\right) \\
&\geq \mathbb{P}\left(\sup_{s\in[0,\, t]} \left|\widetilde{\Theta}^*_s\right| < \epsilon\right).
\end{aligned}$$

But this is positive by the following lemma.

Lemma 4.7. *Brownian motion B_t has a positive probability of being bounded by any positive constant on a finite time interval. That is, for every ϵ, $t > 0$ we have, $P\left(\sup_{s\in[0,\,t]} |B_s| < \epsilon\right) > 0$.*

Proof. Let n be the smallest natural number such that $p := P\left(\sup_{s\in[0,\,t/n]} |B_s| < \epsilon/2\right) > 0$. Such a n exists since otherwise we have

$$0 = \lim_{n\to\infty} P\left(\sup_{s\in[0,\,t/n]} |B_s| < \epsilon/2\right) = P\left(\lim_{n\to\infty} \sup_{s\in[0,\,t/n]} |B_s| < \epsilon/2\right) = P\left(B_0 < \epsilon/2\right) = 1,$$

which is a contradiction. Let m be such that $0 \leq m \leq n-1$. By the Markov property of Brownian motion the event that $|B_s - B_{mt/n}|$ is less than $\epsilon/2$ for $s \in [mt/n, (m+1)t/n]$ has probability p . The event that $B_{(m+1)t/n} - B_{mt/n}$ has the opposite sign to $B_{mt/n}$ has probability $1/2$, by symmetry. By conditioning on that these two events occur for all $m = 0, \ldots, n-1$ we obtain cancellation in such a way that B_s is guaranteed to be bounded by ϵ for all $s \in [0, t]$, that is $P\left(\sup_{s\in[0,\,t]} |B_s| < \epsilon\right) \geq (p/2)^n > 0$. □

Hence (4.15) is false as desired and ϑ_t must be strictly decreasing on $[0, \pi]$.

5

Estimates

In this chapter we establish the following upper bound for the spherical heat kernel

$$K_t^N(\xi,\eta) \lesssim \left(\frac{1}{t+\pi-d(\xi,\eta)}\right)^{\frac{N-1}{2}} \frac{1}{t^{N/2}} \exp\left(-\frac{d(\xi,\eta)^2}{4t}\right), \quad N = 1,2,3, \tag{5.1}$$

for small t. We shall also verify that the estimate is sharp at $d(\xi,\eta)=\pi$, which implies that we cannot set $\delta = 0$ in the estimate (1.2). Note that the upper bound is completely analogous to the Euclidean heat kernel (1.1) up to the factor $(t+\pi-d(\xi,\eta))^{-(N-1)/2}$. For fixed $\xi_0,\eta_0 \in S^N$ which are not antipodal, $d(\xi_0,\eta_0) < \pi$, we see that the factor remains bounded as t gets small so that

$$K_t^N(\xi_0,\eta_0) \simeq \frac{1}{t^{N/2}} \exp\left(-\frac{d(\xi_0,\eta_0)^2}{4t}\right).$$

Note also that the factor reduces to 1 when $N=1$, which means that the spherical heat kernel on S^1 essentially is the same as the Euclidean heat kernel on the real line. For $N = 2,3$ however, the factor increases with the spherical distance and is maximized when the points are antipodal; $d(\xi,\eta)=\pi$. Then, the upper bound suddenly depends on t in another way compared to the Euclidean kernel. Indeed, we have

$$K_t^N(\pi) \simeq \left(\frac{1}{\sqrt{t}}\right)^{N-1} \frac{1}{t^{N/2}} \exp\left(-\frac{\pi^2}{4t}\right). \tag{5.2}$$

It is shown in [8, p. 23] that (5.2) is valid for all N, and it is therefore natural to conjecture that (5.1) also is true for $N > 3$.

5.1 Estimates of K_t^1

Definition 5.1. *For $t > 0$, let $H_t(x)$ be defined by*

$$H_t(x) = \frac{\vartheta_t(x)}{W_t(x)}, \quad x \in [0,\pi].$$

Proposition 5.2. *H_t is strictly increasing and strictly convex on $[0,\pi]$.*

Proof. First we note that H_t can we written in the following way

$$\begin{aligned}
H_t(x) &= \sum_{n\geq 0}\frac{W_t(x+2\pi n)}{W_t(x)}+\sum_{n\leq -1}\frac{W_t(x+2\pi n)}{W_t(x)}\\
&= \sum_{n\geq 0}\frac{W_t(x+2\pi n)}{W_t(x)}+\sum_{n\geq 0}\frac{W_t(x-2\pi(n+1))}{W_t(x)}\\
&= \sum_{n\geq 0}\left[\exp\left(-\frac{\pi^2n^2+\pi x n}{t}\right)+\exp\left(-\frac{\pi^2n^2+(2\pi^2-x\pi)n+\pi^2-\pi x}{t}\right)\right].
\end{aligned}$$

The expression in square brackets is a strictly convex function of x, for all t and n. This implies that H_t is strictly convex. Also, H_t is even since ϑ_t and W_t are even. Therefore, $H_t'(0)=0$ and together with the convexity, this implies that H_t is strictly increasing. □

Proposition 5.3. *For all $\epsilon>0$ there exists $T>0$ such that*

$$H_t(x)\leq 2+\epsilon,\quad x\in[0,\pi],\quad t\in(0,T).$$

Proof. From Proposition 5.2 we have that $H_t(x)\leq H_t(\pi)$ since H_t is increasing. Then we note that

$$\begin{aligned}
H_t(\pi) &= 2\sum_{n\geq 0}\exp\left(-\frac{\pi^2(n^2+n)}{t}\right)\\
&< 2\sum_{n\geq 0}\exp\left(-\frac{2\pi^2 n}{t}\right)\\
&= \frac{2}{1-\exp\left(-\frac{2\pi^2}{t}\right)}.
\end{aligned}$$

So $H_t(\pi)\to 2$ as $t\to 0$, and the result follows.

□

Theorem 5.4. *For sufficiently small t we have*

$$G_t^{-1/2}(\cos\theta,\cos\varphi)\simeq\frac{1}{\sqrt{t}}\exp\left(-\frac{(\theta-\varphi)^2}{4t}\right),\quad \theta,\varphi\in[0,\pi].$$

Proof. From (2.13) we have

$$G_t^{-1/2}(\cos\theta,\cos\varphi)=\vartheta_t(\theta-\varphi)+\vartheta_t(\theta+\varphi).\tag{5.3}$$

By Proposition 5.3 we have that $\vartheta_t\simeq W_t$ for small t. Therefore,

$$\begin{aligned}
G_t^{-1/2}(\cos\theta,\cos\varphi) &\simeq W_t(\theta-\varphi)+W_t(\theta+\varphi)\\
&\simeq \frac{1}{\sqrt{t}}\exp\left(-\frac{(\theta-\varphi)^2}{4t}\right)\left[1+\exp\left(-\frac{\theta\varphi}{t}\right)\right]\\
&\simeq \frac{1}{\sqrt{t}}\exp\left(-\frac{(\theta-\varphi)^2}{4t}\right).
\end{aligned}$$

□

For $\varphi = 0$ we simply get the following corollary which confirms (5.1) for $N = 1$.

Corollary 5.5. *For small* t *we have*

$$K_t^1(\theta) \simeq \frac{1}{\sqrt{t}} \exp\left(-\frac{\theta^2}{4t}\right).$$

5.2 Estimates of K_t^3

Theorem 5.6. *For small* t *we have*

$$K_t^3(\theta) \lesssim \frac{1}{t^{3/2}(\pi - \theta + t)} \exp\left(-\frac{\theta^2}{4t}\right), \quad \theta \in [0, \pi],$$

and the estimate is sharp at $\theta = \pi$*.*

Proof. Recall from Theorem 2.4 that

$$K_t^3(\theta) = \frac{e^t}{2\pi}\left(\frac{-\vartheta_t'(\theta)}{\sin\theta}\right).$$

If we use the fact that $\vartheta_t' = h_t W_t'$ and Corollary 3.5, which states that

$$h_t(\theta) \lesssim \frac{\pi - \theta}{\pi - \theta + t},$$

we obtain,

$$\begin{aligned} K_t^3(\theta) &\lesssim \frac{1}{t^{3/2}(\pi - \theta + t)} \frac{(\pi - \theta)\theta}{\sin\theta} \exp\left(-\frac{\theta^2}{4t}\right) \\ &\simeq \frac{1}{t^{3/2}(\pi - \theta + t)} \exp\left(-\frac{\theta^2}{4t}\right), \end{aligned}$$

as desired. To verify that the estimate is sharp at $\theta = \pi$, we write

$$K_t^3(\pi) \simeq \lim_{\theta \to \pi} \frac{-\vartheta_t'(\theta)}{\sin\theta} = \vartheta''(\pi),$$

and use the fact that $\vartheta_t''(\pi)$ can be written as $2W_t''(\pi)$ plus a sum of terms that that tends to 0 faster than $W_t''(\pi)$ as t gets small. Hence

$$K_t^3(\pi) \simeq W''(\pi) \simeq \frac{1}{t^{5/2}} \exp\left(-\frac{\pi^2}{4t}\right),$$

for small t. □

This theorem confirms (5.1) for $N = 3$.

5.3 Estimates of K_t^2

Lemma 5.7. *Let g be a decreasing integrable function on the interval $[0,a]$. Then*

$$\int_0^a g(x)\frac{1}{\sqrt{x(a-x)}}\,dx \le \frac{2}{\sqrt{a}}\int_0^a g(x)\frac{1}{\sqrt{x}}\,dx.$$

Proof. First we observe that

$$\begin{aligned}\frac{1}{\sqrt{x(a-x)}} &= \frac{1}{\sqrt{x}+\sqrt{a-x}}\left(\frac{1}{\sqrt{x}}+\frac{1}{\sqrt{a-x}}\right)\\ &\le \frac{1}{\sqrt{a}}\left(\frac{1}{\sqrt{x}}+\frac{1}{\sqrt{a-x}}\right).\end{aligned}$$

Thus, it remains to show that

$$\int_0^a g(x)\frac{1}{\sqrt{a-x}}\,dx \le \int_0^a g(x)\frac{1}{\sqrt{x}}\,dx.$$

For arbitrary real numbers $x_2 \ge x_1$ and $y_2 \ge y_1$ one has

$$x_2y_2 + x_1y_1 \ge x_2y_1 + x_1y_2, \tag{5.4}$$

since $(x_2-x_1)(y_2-y_1) \ge 0$. In view of this, we notice that $g(x) \ge g(a-x)$ and $\frac{1}{\sqrt{x}} \ge \frac{1}{\sqrt{a-x}}$ when $x \in [0,a/2]$. Therefore,

$$\begin{aligned}\int_0^a g(x)\frac{1}{\sqrt{a-x}}\,dx &= \int_0^{a/2}\left[g(x)\frac{1}{\sqrt{a-x}}+g(a-x)\frac{1}{\sqrt{x}}\right]dx\\ &\le \int_0^{a/2}\left[g(x)\frac{1}{\sqrt{x}}+g(a-x)\frac{1}{\sqrt{a-x}}\right]dx \qquad \text{by (5.4)}\\ &= \int_0^a g(x)\frac{1}{\sqrt{x}}\,dx,\end{aligned}$$

and we are done. □

It can be interesting to note that the lemma actually is a direct consequence of the Hardy–Littlewood rearrangement inequality, see [5, (378)].

Theorem 5.8. *For small t we have*

$$K_t^2(\theta) \lesssim \frac{1}{t\sqrt{\pi-\theta+t}}\exp\left(-\frac{\theta^2}{4t}\right), \qquad \theta \in [0,\pi],$$

and the estimate is sharp at $\theta = \pi$.

Proof. By Theorem 2.4 and the trigonometric identity

$$\cos a - \cos b = 2\sin\left(\frac{b-a}{2}\right)\sin\left(\frac{b+a}{2}\right),$$

we obtain

$$K_t^2(\theta) \simeq \int_{\theta/2}^{\pi-\theta/2}\frac{-\vartheta'_{t/4}(\gamma)}{\sqrt{\sin\left(\gamma-\frac{\theta}{2}\right)\sin\left(\gamma+\frac{\theta}{2}\right)}}\,d\gamma.$$

Use the relation $\vartheta_t' = h_t W_t'$, and write

$$-\vartheta_{t/4}'(\gamma) \simeq \frac{\gamma}{t^{3/2}} \exp\left(-\frac{\gamma^2}{t}\right) h_{t/4}(\gamma)$$

in the integral, to obtain

$$\frac{1}{t^{3/2}} \int_{\theta/2}^{\pi-\theta/2} \exp\left(-\frac{\gamma^2}{t}\right) \frac{\gamma h_{t/4}(\gamma)}{\sqrt{\sin\left(\gamma - \frac{\theta}{2}\right) \sin\left(\gamma + \frac{\theta}{2}\right)}}\, d\gamma.$$

Make the transformation $\psi = \gamma - \frac{\theta}{2}$ and use the estimate

$$\sin(\psi) \sin(\psi + \theta) \simeq \psi(\pi - \psi)(\psi + \theta)(\pi - \theta - \psi),$$

(which is valid since both ψ and $\psi + \theta$ are in $[0, \pi]$) to obtain

$$K_t^2(\theta) \simeq \frac{1}{t^{3/2}} \exp\left(-\frac{\theta^2}{4t}\right) \int_0^{\pi-\theta} \exp\left(-\frac{\psi^2 + \psi\theta}{t}\right) \frac{\left(\psi + \frac{\theta}{2}\right) h_{t/4}\left(\psi + \frac{\theta}{2}\right)}{\sqrt{\psi(\pi - \psi)(\psi + \theta)(\pi - \theta - \psi)}}\, d\psi. \quad (5.5)$$

Let us denote the integrand in (5.5) by $I_t(\psi, \theta)$. Then it remains to prove that

$$\int_0^{\pi-\theta} I_t(\psi,\theta)\, d\psi \lesssim \frac{\sqrt{t}}{\sqrt{\pi - \theta + t}} \quad (5.6)$$

for all $\theta \in [0, \pi]$. To show this, we consider two cases; when θ is small and large, respectively.

Case 1: Assume that $\theta \in [0, \frac{\pi}{2}]$. It is convenient to factorize the integrand in the following way

$$I_t(\psi, \theta) = \exp\left(-\frac{\psi^2 + \psi\theta}{t}\right) \left[\frac{\psi + \frac{\theta}{2}}{\sqrt{\psi(\psi + \theta)}}\right] \left[\frac{h_{t/4}(\psi + \frac{\theta}{2})}{\sqrt{(\pi - \psi)(\pi - \psi - \theta)}}\right]. \quad (5.7)$$

Then the two factors in square brackets in (5.7) are bounded on $\psi \in [\frac{\pi}{4}, \pi - \theta]$ and $\psi \in [0, \frac{\pi}{4}]$, respectively. That is,

$$\sup\left\{\frac{\psi + \frac{\theta}{2}}{\sqrt{\psi(\psi + \theta)}} : \theta \in \left[0, \frac{\pi}{2}\right], \psi \in \left[\frac{\pi}{4}, \pi - \theta\right]\right\} \simeq 1 \quad (5.8)$$

and (recall $h_{t/4} \leq 1$ by Lemma 3.4)

$$\sup\left\{\frac{h_{t/4}(\psi + \frac{\theta}{2})}{\sqrt{(\pi - \psi)(\pi - \psi - \theta)}} : \theta \in \left[0, \frac{\pi}{2}\right], \psi \in \left[0, \frac{\pi}{4}\right]\right\} \simeq 1. \quad (5.9)$$

But the two factors are unbounded on $\psi \in [0, \frac{\pi}{4}]$ and $\psi \in [\frac{\pi}{4}, \pi - \theta]$, respectively. And when this is the case, we shall use the following estimates

$$\frac{\psi + \frac{\theta}{2}}{\sqrt{\psi(\psi + \theta)}} \simeq \sqrt{\frac{\psi}{\psi + \theta}} + \sqrt{\frac{\theta}{\psi}} \lesssim 1 + \sqrt{\frac{\theta}{\psi}}, \quad (5.10)$$

and

$$\begin{aligned}
\frac{h_{t/4}(\psi+\frac{\theta}{2})}{\sqrt{(\pi-\psi)(\pi-\psi-\theta)}} &\leq \frac{h_{t/4}(\psi)}{\sqrt{\pi-\psi}}\frac{1}{\sqrt{\pi-\psi-\theta}} \quad \text{since } h_t \text{ is decreasing} \\
&\leq \min\left(\frac{1}{\sqrt{\pi-\psi}}, \frac{4\pi}{t}\sqrt{\pi-\psi}\right)\frac{1}{\sqrt{\pi-\psi-\theta}} \quad \text{by Lemma 3.4.} \\
&\leq \sqrt{\frac{4\pi}{t}}\frac{1}{\sqrt{\pi-\psi-\theta}}. \qquad (5.11)
\end{aligned}$$

The analysis done so far motivates us to break up the integral as follows:

$$\int_0^{\pi-\theta} I_t(\psi,\theta)\,d\psi = \int_0^{\pi/4} I_t(\psi,\theta)\,d\psi + \int_{\pi/4}^{\pi-\theta} I_t(\psi,\theta)\,d\psi.$$

For the first integral we have

$$\begin{aligned}
\int_0^{\pi/4} I_t(\psi,\theta)\,d\psi &\lesssim \int_0^{\pi/4} \exp\left(-\frac{\psi^2+\psi\theta}{t}\right)\left[1+\sqrt{\frac{\theta}{\psi}}\right]d\psi \quad \text{by (5.9) and (5.10)} \\
&\leq \int_0^{\pi/4} \exp\left(-\frac{\psi^2}{t}\right)d\psi + \int_0^{\pi/4}\sqrt{\frac{\theta}{\psi}}\exp\left(-\frac{\psi\theta}{t}\right)d\psi \\
&\leq \sqrt{t}\left(\int_0^\infty e^{-x^2}\,dx + \int_0^\infty \frac{1}{\sqrt{y}}e^{-y}\,dy\right) \simeq \sqrt{t}.
\end{aligned}$$

For the second integral we have

$$\begin{aligned}
\int_{\pi/4}^{\pi-\theta} I_t(\psi,\theta)\,d\psi &\lesssim \int_{\pi/4}^{\pi-\theta} \exp\left(-\frac{\psi^2}{t}\right)\left[\sqrt{\frac{4\pi}{t}}\frac{1}{\sqrt{\pi-\psi-\theta}}\right]d\psi \quad \text{by (5.8) and (5.11)} \\
&\leq \exp\left(-\frac{\pi^2}{16t}\right)\sqrt{\frac{4\pi}{t}}\int_{\pi/4}^{\pi-\theta}\frac{1}{\sqrt{(\pi-\psi-\theta)}}\,d\psi \\
&\leq \exp\left(-\frac{\pi^2}{16t}\right)2\pi\sqrt{\frac{3}{t}} \quad \leq \sqrt{t}, \quad \text{for small } t.
\end{aligned}$$

By adding up the two previous results we infer

$$\int_0^{\pi-\theta} I_t(\psi,\theta)\,d\psi \lesssim \sqrt{t}, \quad \theta \in \left[0, \frac{\pi}{2}\right], \qquad \text{for small } t,$$

which implies that (5.6) is true for $\theta \in \left[0, \frac{\pi}{2}\right]$. Thus it remains to prove (5.6) for the second case, when $\theta \in [\frac{\pi}{2}, \pi]$.

Case 2: Assume that $\theta \in [\frac{\pi}{2}, \pi]$. In this case, it is convenient to factorize the integrand $I_t(\theta,\psi)$ in the following way

$$I_t(\theta,\psi) = \exp\left(-\frac{\psi^2+\psi\theta}{t}\right)\frac{1}{\sqrt{\psi(\pi-\theta-\psi)}}\left[\frac{\left(\psi+\frac{\theta}{2}\right)h_{t/4}\left(\psi+\frac{\theta}{2}\right)}{\sqrt{(\pi-\psi)(\psi+\theta)}}\right].$$

Then we observe that the expression in square brackets is bounded for $\theta \in \left[\frac{\pi}{2}, \pi\right]$ and the interval of integration $\psi \in [0, \pi-\theta]$,

$$\sup\left\{\frac{\left(\psi+\frac{\theta}{2}\right)h_{t/4}\left(\psi+\frac{\theta}{2}\right)}{\sqrt{(\pi-\psi)(\psi+\theta)}} : \theta \in \left[\frac{\pi}{2}, \pi\right], \psi \in [0, \pi-\theta]\right\} \simeq 1.$$

From this observation we conclude that

$$\int_0^{\pi-\theta} I_t(\theta,\psi)\, d\psi \simeq \int_0^{\pi-\theta} \exp\left(-\frac{\psi\theta}{t}\right) \frac{1}{\sqrt{\psi(\pi-\theta-\psi)}}\, d\psi. \tag{5.12}$$

Make the transformation $\psi = (\pi-\theta)x$ and use Lemma (5.7) to get

$$\simeq \int_0^1 \exp\left(-\theta\frac{(\pi-\theta)x}{t}\right) \frac{1}{\sqrt{x}}\, dx.$$

Make the transformation $\omega = (\pi-\theta)x/t$ to obtain

$$\frac{\sqrt{t}}{\sqrt{\pi-\theta}} \int_0^{\frac{\pi-\theta}{t}} \frac{1}{\sqrt{\omega}} e^{-\theta\omega}\, d\omega \tag{5.13}$$

Since $\theta \geq \pi/2$, the integrand is integrable on $[0,\infty]$, which implies that the integral is less than a positive constant. Hence

$$\int_0^{\pi-\theta} I_t(\theta,\psi)\, d\psi \lesssim \frac{\sqrt{t}}{\sqrt{\pi-\theta}}. \tag{5.14}$$

From (5.12) we also obtain

$$\int_0^{\pi-\theta} I_t(\theta,\psi)\, d\psi \lesssim \int_0^{\pi-\theta} \frac{1}{\sqrt{\psi(\pi-\theta-\psi)}}\, d\psi \simeq 1. \tag{5.15}$$

If we combine (5.14) and (5.15) we infer that

$$\begin{aligned} \int_0^{\pi-\theta} I_t(\theta,\psi)\, d\psi &\lesssim \min\left(\frac{\sqrt{t}}{\sqrt{\pi-\theta}}, 1\right) \\ &= \sqrt{t}\min\left(\frac{1}{\sqrt{\pi-\theta}}, \frac{1}{\sqrt{t}}\right) \\ &\lesssim \frac{\sqrt{t}}{\sqrt{\pi-\theta+t}}, \end{aligned}$$

which proves (5.6) for the case when $\theta \in \left[\frac{\pi}{2}, \pi\right]$ and thereby completes the proof of the estimate. To verify that the estimate is sharp at $\theta = \pi$, we use (2.33) and (2.32) to obtain

$$K_t^2(\pi) = \frac{1}{8\pi}\int_{-1}^1 G_{t/4}^{1/2}(0,1) \frac{1}{\sqrt{1-v^2}}\, dv \simeq G_{t/4}^{1/2}\left(\cos\frac{\pi}{2}, 1\right) \simeq -\vartheta'_{t/4}(\pi/2).$$

If we use the relation $\vartheta'_{t/4}(\pi/2) = h_{t/4}(\pi/2)W'_{t/4}(\pi/2)$ and the fact that $h_{t/4}(\pi/2) \simeq 1$ for small t (since $h_{t/4}$ is concave on $[0,\pi]$ for small t by Theorem 3.2), we conclude

$$K_t^2(\pi) \simeq W'_{t/4}(\pi/2) \simeq \frac{1}{t^{3/2}} \exp\left(-\frac{\pi^2}{4t}\right).$$

□

This theorem confirms (5.1) for $N = 2$.

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