Heat Semigroups and Diffusion of Characteristic Functions

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Contents

Introduction

We start from a uniform distribution of heat in a compact subset D of $\mathbb{R}^n$ represented by the characteristic function $\mathbb{1}_D$ of D. Then the heat semigroup $(T(t))_{t\geq 0}$ on $L^2(\mathbb{R}^n)$, applied to $\mathbb{1}_D$, gives the unique solution $u(x,t) = T(t)\mathbb{1}_D(x)$ of the heat equation

$$\text{(HE)} \qquad \begin{cases} \frac{d}{dt}u(x,t) = \Delta u(x,t), & x \in \mathbb{R}^n, t \geq 0, \\ u(x,0) = \mathbb{1}_D(x) \end{cases}$$

on $\mathbb{R}^n$ for all times $t \geq 0$ with initial data $\mathbb{1}_D$.
This heat flow in particular induces an evolution of the corresponding L^2-norms

$$t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \geq 0. \tag{1}$$

If we adopt the notation

$$\langle f, g\rangle := \int_{\mathbb{R}^n} f(x) \cdot g(x)\, dx$$

both for the inner product on $L^2(\mathbb{R}^n)$ and for the duality pairing $\langle L^1(\mathbb{R}^n), L^\infty(\mathbb{R}^n)\rangle$, then by the semigroup property

$$T(t+s)\mathbb{1}_D = T(t)T(s)\mathbb{1}_D, \qquad s,t \geq 0$$

and the self-adjointness of the operators $T(t)$ we obtain the following alternative description for the evolution (1):

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = \langle T(\tfrac{t}{2})\mathbb{1}_D, T(\tfrac{t}{2})\mathbb{1}_D\rangle = \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2, \qquad t \geq 0. \tag{2}$$

Since on $\mathbb{R}^n$ no heat is lost under diffusion, this also yields

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = |D| - \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = |D| - \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2, \quad t \geq 0. \tag{3}$$

Observe that, by

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = \int_D T(t)\mathbb{1}_D(x)\, dx \quad \text{and} \quad \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = \int_{D^c} T(t)\mathbb{1}_D(x)\, dx,$$

(2) describes the amount of heat that is, at time t, still inside the set D, while (3) describes the heat that has flowed into the complement D^c. In this sense the evolution of the L^2-norm (1) directly reflects how good the set D keeps the heat inside.

M. Ledoux [Led94] discovered that there are interesting connections between the heat flow into the complement (3) and the perimeter $P(D)$ of D, i.e., area measure of the boundary ∂D in the sense of geometric measure theory. In particular he proved that the L^2-inequality

$$\|T(t)\mathbb{1}_D\|_{L^2} \le \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t \ge 0, \tag{4}$$

for a Euclidean ball B and a second compact set D of the same volume implies the isoperimetric inequality

$$P(D) \ge P(B),$$

i.e., the Euclidean ball has the smallest perimeter under all compact sets of the same volume.
This is in fact a very interesting conclusion since the L^2-inequality (4) can be derived easily from the Riesz-Sobolev inequality for symmetric rearrangements in $\mathbb{R}^n$, a fact that, remarkably, was not realized by Ledoux.

In this thesis we present a further systematic treatment of the connections between properties of the heat flow (1)-(3) and the geometry of D. Our main results concern the short time behaviour as well as large time phenomena.

In the *first chapter* we give a brief summary of the analytic and geometric concepts and results that will be used in the following. We introduce the heat semigroup on $\mathbb{R}^n$ and its main properties. We recall the concept of symmetric rearrangements in $\mathbb{R}^n$, the Riesz-Sobolev inequality and present the interesting, but rather unknown, connections between the heat semigroup and rearrangement inequalities. These connections then lead to a proof of the isoperimetric inequality. Further, we briefly present the necessary background on perimeters, relevant geometric measure theory and the basic notions of the geometry of smooth hypersurfaces in $\mathbb{R}^n$.

In *Chapter two* we focus on the short time behaviour of the flow $t \mapsto T(t)\mathbb{1}_D$. We start with a detailed treatment of the evolution of the level sets of $T(t)\mathbb{1}_D$ and determine the pointwise asymptotic behaviour for this evolution: We show that for short times the evolution of the level sets admits an asymptotic expansion in powers of $t^{1/2}$. We determine the coefficients up to order t^2 in terms of geometric invariants of the boundary ∂D and give a general formula for the further coefficients of higher order.
We then show that the short time behaviour of the flow (1)-(3) is controlled by the perimeter of D. We prove this first for a compact set with smooth boundary using the results obtained for the evolution of the level sets, and then for a Caccioppoli set using measure theoretic arguments. These results generalise what Ledoux [Led94] proved for Euclidean balls.
As a consequence we obtain a comparison result stating that for two arbitrary compact sets $A, D \subset \mathbb{R}^n$ of the same volume the one with smaller perimeter keeps for small times the heat better than the other - a fact that corresponds to the isoperimetric character of inequality (4) but now allows to compare two arbitrary compact sets of the same volume and not only the Euclidean ball and a second set.

In the *third chapter* we concentrate on large time phenomena of the flow (1)-(3). In particular, we study the analogue of the question treated at the end of Chapter 2: Given two compact sets $A, D \subset \mathbb{R}^n$ of the same volume. Which one keeps the heat better for large times? We again prove a comparison theorem stating now that this holds for the one which has the smaller second central moment. This again compatibly corresponds to the inequality (4) since the Euclidean ball minimizes the second central moment under all sets of a given volume.
In addition we give further criteria on the fourth central moments and on the tensors of inertia of A and D yielding an answer in case the second central moments are equal.

We conclude with considerations on the question how much geometry of D is already determined if we know the flow (1)-(3) on a (maybe small) time interval.

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Chapter 1

Heat diffusion and the isoperimetric inequality

In this chapter we give a short summary of the notions and results we frequently need in the following. We introduce the heat semigroup (Section 1.1), symmetric rearrangements of sets and functions, the Riesz-Sobolev inequality (Section 1.2), perimeter, some measure theoretic background (Section 1.3), connections between the heat semigroup and the isoperimetric inequality (Section 1.4), and finally the basic notions of the geometry of smooth hypersurfaces in $\mathbb{R}^n$ (Section 1.5).

1.1 The heat semigroup

We consider the heat equation (HE) in $\mathbb{R}^n$

$$\text{(HE)} \qquad \begin{cases} \frac{d}{dt}u(x,t) = \Delta u(x,t), & x \in \mathbb{R}^n, t \geq 0, \\ u(x,0) = \mathbb{1}_D(x), & \end{cases}$$

where the Laplace operator $\Delta : D(\Delta) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is given by

$$\begin{aligned} \Delta u(x,t) &= \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} u(x_1, ..., x_n, t) \qquad \text{with domain} \\ D(\Delta) &= W^{2,2}(\mathbb{R}^n), \end{aligned}$$

and where $\mathbb{1}_D \in L^2(\mathbb{R}^n)$ denotes the characteristic function of a compact set $D \subset \mathbb{R}^n$.

Using, e.g., the Fourier transform we obtain that the Laplace operator $(\Delta, W^{2,2}(\mathbb{R}^n))$ generates a strongly continuous, analytic semigroup $(T(t))_{t\geq 0}$ of linear operators, the *heat semigroup*, on $L^2(\mathbb{R}^n)$. This semigroup is given explicitly by the integral kernel

$$p(x,y,t) = \frac{1}{(4\pi t)^{n/2}} e^{\frac{-|x-y|^2}{4t}}, \qquad x, y \in \mathbb{R}^n, t > 0,$$

called the *Gauß-Weierstrass kernel* or simply the *heat kernel* on $\mathbb{R}^n$, and provides the unique solution of (HE):

$$
\begin{aligned}
u(t,x) = T(t)\mathbb{1}_D(x) &= \int_{\mathbb{R}^n} p(x,y,t)\,\mathbb{1}_D(y)\,dy \\
&= \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{\frac{-|x-y|^2}{4t}} \mathbb{1}_D(y)\,dy \\
&= \frac{1}{(4\pi t)^{n/2}} \int_D e^{\frac{-|x-y|^2}{4t}}\,dy, \qquad x \in \mathbb{R}^n, t > 0.
\end{aligned}
$$

Physically speaking, $u(t,x)$ describes the heat flow we obtain if at time $t = 0$ the heat is distributed uniformly in the set D and no heat is in the complement of D. Then the function $T(t)\mathbb{1}_D$ yields the distribution of heat at time t.

If one studies the behaviour of the solution $t \mapsto T(t)\mathbb{1}_D$ and in particular the evolution of the L^2-norms $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$ for a given compact set $D \subset \mathbb{R}^n$, one expects that it should be closely related to geometric properties of D, such as its volume, its perimeter and other geometric and/or physical quantities.

Let us further recall the main properties of the heat semigroup $(T(t))_{t\geq 0}$ and in particular the relations between properties of the operator $T(t)$ and properties of the kernel $p(x,y,t)$.

i) Symmetry of kernel and semigroup

The Gauß-Weierstrass kernel

$$
p(x,y,t) = \frac{1}{(4\pi t)^{n/2}}\, e^{\frac{-|x-y|^2}{4t}}
$$

is symmetric with respect to the two space variables $x, y \in \mathbb{R}^n$. By Fubini's Theorem this corresponds to the symmetry of the operator $T(t)$ on $L^2(\mathbb{R}^n)$ by

$$
\begin{aligned}
\langle T(t)\mathbb{1}_A, \mathbb{1}_D\rangle_{L^2} &= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} p(x,y,t)\mathbb{1}_A(y)\,dy\,\mathbb{1}_D(x)\,dx \\
&= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} p(x,y,t)\,\mathbb{1}_A(y)\,\mathbb{1}_D(x)\,dy\,dx \\
&= \int_{\mathbb{R}^n} \mathbb{1}_A(y) \int_{\mathbb{R}^n} p(x,y,t)\,\mathbb{1}_D(x)\,dx\,dy \\
&= \langle \mathbb{1}_A, T(t)\mathbb{1}_D\rangle_{L^2}, \qquad t > 0.
\end{aligned}
$$

ii) Semigroup property

Furthermore, the semigroup property

$$
T(t+s)\mathbb{1}_D = T(t)T(s)\mathbb{1}_D, \qquad s,t > 0,
$$

is reflected by the well-known "semigroup formula" for the kernel

$$p(x,y,t+s) = \int_{\mathbb{R}^n} p(x,z,t)p(z,y,s)\,dz, \qquad x,y\in\mathbb{R}^n,\ s,t>0.$$

In fact, it holds that

$$\begin{aligned} T(t)T(s)\mathbb{1}_D(x) &= \int_{\mathbb{R}^n} p(z,x,t)\Big(T(s)\mathbb{1}_D(z)\Big)\,dz \\ &= \int_{\mathbb{R}^n} p(z,x,t)\int_{\mathbb{R}^n} p(z,y,s)\,\mathbb{1}_D(y)\,dy\,dz \\ &= \int_{\mathbb{R}^n} \underbrace{\int_{\mathbb{R}^n} p(x,z,t)p(z,y,s)\,dz}_{=p(x,y,t+s)}\,\mathbb{1}_D(y)\,dy \\ &= \int_{\mathbb{R}^n} p(x,y,t+s)\,\mathbb{1}_D(y)\,dy \\ &= T(t+s)\mathbb{1}_D(x). \end{aligned}$$

iii) Relation between norm and inner product

Now the symmetry and semigroup properties of the operators $T(t)$ yield an elementary but important relation between the norm and the inner product on the Hilbert space $L^2(\mathbb{R}^n)$. Indeed, we have the following identities

$$\begin{aligned} \|T(\tfrac{t}{2})\mathbb{1}_D\|^2_{L^2} &= \langle T(\tfrac{t}{2})\mathbb{1}_D, T(\tfrac{t}{2})\mathbb{1}_D\rangle_{L^2} = \langle T(\tfrac{t}{2})T(\tfrac{t}{2})\mathbb{1}_D, \mathbb{1}_D\rangle_{L^2} \\ &= \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle_{L^2} = \int_D T(t)\mathbb{1}_D(x)\,dx, \qquad t\geq 0, \end{aligned} \tag{1.1}$$

i.e., the square of the L^2-norm of the evolution $t\mapsto T(t)\mathbb{1}_D$ at time $\frac{t}{2}$ is equal to the amount of heat that is still inside D after time t.

Further the map $t\mapsto \|T(t)\mathbb{1}_D\|^2_{L^2}$ has the following properties.

Proposition 1. *Let $D\subset\mathbb{R}^n$ be a compact set. Then the map*

$$t\mapsto \|T(t)\mathbb{1}_D\|^2_{L^2}, \qquad t\geq 0,$$

is strictly decreasing and strictly convex.

Proof: The first derivative of $\|T(t)\mathbb{1}_D\|_{L^2}^2$ satisfies

$$\begin{aligned}\frac{d}{dt}\|T(t)\mathbb{1}_D\|_{L^2}^2 &= \frac{d}{dt}\langle T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle \\ &= 2\,\langle \frac{d}{dt}T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle \\ &= 2\,\langle \Delta T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle \\ &= 2\int_{\mathbb{R}^n} \Delta T(t)\mathbb{1}_D(x)\cdot T(t)\mathbb{1}_D(x)\,dx \\ &= -2\int_{\mathbb{R}^n} |\nabla T(t)\mathbb{1}_D(x)|^2\,dx < 0,\end{aligned}$$

so $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}^2$ is strictly decreasing. Furthermore

$$\begin{aligned}\frac{d^2}{dt^2}\|T(t)\mathbb{1}_D\|_{L^2}^2 &= \frac{d}{dt}\,2\,\langle \Delta T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle \\ &= 2\,\langle \frac{d}{dt}\Delta T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle + 2\,\langle \Delta T(t)\mathbb{1}_D, \frac{d}{dt}T(t)\mathbb{1}_D\rangle \\ &= 2\,\langle \Delta\frac{d}{dt}T(t)\mathbb{1}_D, T(t)\mathbb{1}_D\rangle + 2\,\langle \Delta T(t)\mathbb{1}_D, \Delta T(t)\mathbb{1}_D\rangle \\ &= 4\,\langle \Delta T(t)\mathbb{1}_D, \Delta T(t)\mathbb{1}_D\rangle > 0,\end{aligned}$$

so $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}^2$ is strictly convex. □

Remark 2. Note that, since the heat semigroup $(T(t))_{t\geq 0}$ is analytic on $L^2(\mathbb{R}^n)$, also the map

$$t \mapsto \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle_{L^2} = \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2$$

is analytic for $t \in (0,\infty)$. So in particular we obtain that for two different compact sets $A, D \subset \mathbb{R}^n$ the maps

$$t \mapsto \|T(t)\mathbb{1}_A\|_{L^2} \quad \text{and} \quad t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$$

coincide everywhere if they coincide on an arbitrarily small time interval or even on a sequence $(t_n)_{n\in\mathbb{N}}$ with accumulation point in $(0,\infty)$.

1.2 Symmetric rearrangements, the Riesz-Sobolev inequality and an L^2-diffusion inequality

We now introduce the notion of symmetric rearrangements in $\mathbb{R}^n$ and give a short overview of the results we need. Most of the material is taken from [LL95], but see also [Bae94], [Cha01], [HLP52].

In the second part of this section we deduce a very useful L^2-diffusion inequality.

General background

We start with the symmetric rearrangement of sets.

Definition 3. (Rearrangement of sets) Let $D \subset \mathbb{R}^n$ be a compact set. We define the *symmetric rearrangement* D^* of D to be the closed Euclidean ball centered at the origin which has the same volume as D:

$$D^* := B_r(0) = \{x \in \mathbb{R}^n : |x| \leq r\} \qquad \text{with } r = \left(\frac{|D|}{\omega_n}\right)^{1/n},$$

where $\omega_n = |\mathbb{B}^n|$ is the volume of the n-dimensional Euclidean unit ball.

The procedure to define the *symmetric-decreasing rearrangement* of a characteristic function is quite intuitive and one simply sets

$$\mathbb{1}^*_D := \mathbb{1}_{D^*}.$$

This allows us to define the rearrangement of more general functions $f : \mathbb{R}^n \to \mathbb{R}$.
We call a measurable function $f : \mathbb{R}^n \to \mathbb{R}$ *vanishing at infinity* if the superlevel sets of $|f|$, i.e., the sets

$$\{x \in \mathbb{R}^n : |f(x)| \geq \lambda\}$$

have finite measure for all $\lambda \in (0, \infty)$.
The main idea to define the *symmetric-decreasing rearrangement* for such f is now that the superlevel sets of f^* should be the rearrangements of the level sets of $|f|$, namely

$$\{x \in \mathbb{R}^n : |f(x)| \geq \lambda\}^* = \{x \in \mathbb{R}^n : f^*(x) \geq \lambda\}, \qquad \lambda \in (0, \infty).$$

This is expressed as follows.

Definition 4. (Rearrangement of functions) Let $f : \mathbb{R}^n \to \mathbb{R}$ be a measurable function vanishing at infinity. The *symmetric-decreasing rearrangement* f^* of f is defined by

$$f^*(x) := \int_0^\infty \mathbb{1}^*_{\{x \in \mathbb{R}^n : |f(x)| \geq \lambda\}}(x)\, d\lambda, \qquad x \in \mathbb{R}^n.$$

The definition directly yields that the function $f^* : \mathbb{R}^n \to \mathbb{R}$ has the following nice properties:

(i) f^* is positive,
(ii) f^* is radially symmetric with respect to the origin,
(iii) f^* decreases as $|x|$ increases,
(iv) if $f \in L^p(\mathbb{R}^n)$, then also $f^* \in L^p(\mathbb{R}^n)$ and $\|f\|_{L^p} = \|f^*\|_{L^p}$.

Besides these immediate properties of the function f^*, there are many useful and nontrivial inequalities comparing integrals of functions before and after symmetric-decreasing rearrangement. For a whole variety of these inequalities one should consult, e.g., [LL97], [Bae94], [Bur96].

Probably the most famous inequality for symmetric-decreasing rearrangements is the so called *Riesz-Sobolev inequality.* It was first proved in dimension $n = 1$ by F. Riesz [Rie30] and in arbitrary dimensions by S.L. Sobolev [Sob38], [Sob63]. For a modern proof we refer e.g. to [LL97, Theorem 3.7].

Theorem 5 (Riesz-Sobolev inequality). *Let f, g, h be three positive functions on $\mathbb{R}^n$ vanishing at infinity. Then it holds that*

$$\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} f(x)\, g(x-y)\, h(y)\, dx\, dy \le \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} f^*(x)\, g^*(x-y)\, h^*(y)\, dx\, dy, \tag{1.2}$$

i.e., under symmetric-decreasing rearrangement the value of the double integral does never decrease.

For the interesting history of this inequality and the question of finding cases of equality we refer to [Bur96] and the references therein. Under strong conditions on g the following holds.

Theorem 6. *Let f, g, h be three nonnegative functions on $\mathbb{R}^n$ such that $g(x-y) = g^*(x-y)$ and g is* strictly *decreasing. Then one has equality in (1.2) if and only if*

$$f(x) = f^*(x-y) \quad \text{and} \quad h(x) = h^*(x-y) \qquad \text{for some } y \in \mathbb{R}^n,$$

i.e., only if the functions f, h are already symmetric up to an eventual translation by $y \in \mathbb{R}^n$.

For the proof we again refer to [LL97, Theorem 3.9].

The Riesz-Sobolev inequality as an L^2-diffusion inequality

As a very useful application of the Riesz-Sobolev inequality we now obtain the following L^2-diffusion inequality for characteristic functions which will have far reaching consequences. Although the following considerations are quite natural, we could not find them explicitly in the literature.

Theorem 7 (L^2-diffusion inequality). *Let $D, B \subset \mathbb{R}^n$ be compact sets of the same volume and B a Euclidean ball. Then it holds that*

$$\|T(t)\mathbb{1}_D\|_{L^2} \le \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t \ge 0. \tag{1.3}$$

Further, for $t > 0$ equality holds if and only if D is also a Euclidean ball. So if D is not a ball, one has

$$\|T(t)\mathbb{1}_D\|_{L^2} < \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t > 0. \tag{1.4}$$

Proof: By

$$\|T(0)\mathbb{1}_D\|_{L^2} = \|\mathbb{1}_D\|_{L^2} = \Big(\int_{\mathbb{R}^n} |\mathbb{1}_D(x)|^2\, dx\Big)^{1/2} = |D|^{1/2}$$

and condition $|D| = |B|$ one always has equality in (1.3) for $t = 0$.
For some fixed $t > 0$ we now apply the Riesz-Sobolev inequality to the characteristic function $\mathbb{1}_D$ and the Euclidean heat kernel $p(x, y, t)$, i.e., we take

$$f = h = \mathbb{1}_D \qquad \text{and}$$
$$g(x-y) = p(x,y,t) = \frac{1}{(4\pi t)^{n/2}}\, e^{\frac{-|x-y|^2}{4t}}.$$

Observe that, since $p(x, y, t)$ is positive, radially symmetric and decreasing with respect to the difference $x - y \in \mathbb{R}^n$, it coincides with its symmetric-decreasing rearrangement: $p(x, y, t) = p^*(x, y, t)$.

Further we may assume that the ball B is centered at the origin. Then with $\mathbb{1}^*_D = \mathbb{1}_B$ we obtain the following inequality valid for every $t > 0$

$$\begin{aligned}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \mathbb{1}_D(x)\, p(x,y,t)\, \mathbb{1}_D(y)\, dx\, dy &\leq \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \mathbb{1}^*_D(x)\, p(x,y,t)\, \mathbb{1}^*_D(y)\, dx\, dy \\ &= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \mathbb{1}_B(x)\, p(x,y,t)\, \mathbb{1}_B(y)\, dx\, dy. \qquad (1.5)\end{aligned}$$

Note now that

$$\begin{aligned}\int_{\mathbb{R}^n}\int_{\mathbb{R}^n} \mathbb{1}_D(x)\, p(x,y,t)\, \mathbb{1}_D(y)\, dx\, dy &= \int_{\mathbb{R}^n} \mathbb{1}_D(y) \int_{\mathbb{R}^n} \mathbb{1}_D(x)\, p(x,y,t)\, dx\, dy \\ &= \int_{\mathbb{R}^n} \mathbb{1}_D(y) \cdot T(t)\mathbb{1}_D(y)\, dy \\ &= \langle \mathbb{1}_D, T(t)\mathbb{1}_D \rangle_{L^2} \\ &= \|T(\tfrac{t}{2})\mathbb{1}_D\|^2_{L^2}\end{aligned}$$

by the semigroup property and symmetry of $T(t)$, see (1.1). Therefore, inequality (1.5) is equivalent to

$$\|T(\tfrac{t}{2})\mathbb{1}_D\|^2_{L^2} \leq \|T(\tfrac{t}{2})\mathbb{1}_B\|^2_{L^2}, \qquad t > 0,$$

i.e., equivalent to

$$\|T(t)\mathbb{1}_D\|_{L^2} \leq \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t > 0.$$

This together with the equality for $t = 0$ proves (1.3).

Further note that for every $t > 0$ the heat kernel $p(x, y, t)$ is *strictly* decreasing as the difference $x - y \in \mathbb{R}^n$ increases. Then by Theorem 6 one can have equality in (1.3) for $t > 0$ only if $\mathbb{1}_D = \mathbb{1}^*_D$, i.e., only if D is already a ball. □

Remark 8. One of the distinctive properties of the above inequality (1.3) is that it holds for *all* times t. When we compare the L^2-norms for two *arbitrary* compact sets $A, D \subset \mathbb{R}^n$ of the same volume (cf. Chapter 2 and 3), we see that it is a very special case to have the L^2-inequality for all t. In general, opposite inequality signs may occur for short and for large times.

1.3 Functions of bounded variation, perimeter and measure theoretic notions

We recall the following important definition, see e.g. [AFP00], [BZ88], [EG92], [Giu84].

Definition 9. We say that $f \in L^1(\mathbb{R}^n)$ has *bounded variation* on $\mathbb{R}^n$ if

$$\int_{\mathbb{R}^n} |Df| := \sup\Big\{ \int_{\mathbb{R}^n} f \operatorname{div} g \, dx : g \in C_0^1(\mathbb{R}^n, \mathbb{R}^n), |g| \le 1 \Big\} < \infty$$

and write $f \in BV(\mathbb{R}^n)$.

Using characteristic functions we define the perimeter of a set in the following way (see e.g. also the original work of E. de Giorgi [DG53]).

Definition 10. Let $A \subset \mathbb{R}^n$ be a measurable set with finite volume. We define the *perimeter of* A to be the variation of the characteristic function $\mathbb{1}_A$ in $\mathbb{R}^n$,

$$P(A) := \int_{\mathbb{R}^n} |D\mathbb{1}_A| = \sup\Big\{ \int_{\mathbb{R}^n} \mathbb{1}_A \operatorname{div} g \, dx : g \in C_0^1(\mathbb{R}^n, \mathbb{R}^n), |g| \le 1 \Big\}.$$

The set $A \subset \mathbb{R}^n$ is called a *Caccioppoli set* if $P(A) < \infty$.

Further we denote by $\mathcal{H}^k(A), 1 \le k \le n$, the k-dimensional Hausdorff measure of a subset $A \subset \mathbb{R}^n$ (which coincides with the classical measure for k-dimensional smooth submanifolds).
For sets $A \subset \mathbb{R}^n$ with a Lipschitz boundary ∂A one can show that

$$P(A) = \mathcal{H}^{n-1}(\partial A)$$

(see e.g. [EG92, p. 183f]).
For a measure μ and a measurable set A, we define by $\mu \llcorner A$ the *restriction measure*, i.e.,

$$\mu \llcorner A(D) := \mu(A \cap D)$$

for all measurable sets D.

Definition 11. For a measurable set A and $t \in [0,1]$ we denote by A^t the set

$$A^t := \Big\{ x \in \mathbb{R}^n : \lim_{r \to 0} \frac{|A \cap B_r(x)|}{|B_r|} = t \Big\}. \tag{1.6}$$

This set is called the *set of points of density* t and we define the *essential boundary* (often also called the *measure theoretic boundary*) of A as

$$\partial^* A := \mathbb{R}^n \setminus (A^0 \cup A^1).$$

The *reduced boundary* $\mathcal{F}A$ of A is defined as follows: If $A \subset \mathbb{R}^n$ is a Caccioppoli set, then $x \in \operatorname{supp}|D\mathbb{1}_A|$ belongs to $\mathcal{F}A$ if the limit

$$\nu_A(x) := \lim_{r\to 0} \frac{D\mathbb{1}_A(B_r(x))}{|D\mathbb{1}_A|(B_r(x))}$$

exists in $\mathbb{R}^n$ and satisfies $|\nu_A(x)| = 1$. The map $\nu_A : \mathcal{F}A \to S^{n-1}$ is called the *generalised (or measure theoretic) inner normal* to A, and (see e.g. [AFP00, Theorem 3.59]) for every $x \in \mathcal{F}A$ the hyperplane $\pi_x = \{y \in \mathbb{R}^n : \langle y, \nu_A(x)\rangle = 0\}$ is the *approximate tangent space* to $\mathcal{F}A$ at x.

Moreover (see e.g. [AFP00, Theorem 3.78]), it holds that

$$\mathcal{H}^{n-1}(\partial^* A \setminus \mathcal{F}A) = 0 \tag{1.7}$$

and

$$\mathcal{H}^{n-1}(\mathbb{R}^n \setminus [(A^0 \cup A^1) \cup \mathcal{F}A]) = 0. \tag{1.8}$$

Thus the distributional derivative of $\mathbb{1}_A$ is given by the $\mathbb{R}^n$-valued measure

$$D\mathbb{1}_A = \nu_A \mathcal{H}^{n-1} \llcorner \mathcal{F}A. \tag{1.9}$$

Further

$$|D\mathbb{1}_A| = \mathcal{H}^{n-1} \llcorner \mathcal{F}A, \tag{1.10}$$

and in particular

$$P(A) = \mathcal{H}^{n-1}(\mathcal{F}A). \tag{1.11}$$

As a consequence, for Caccioppoli sets a *generalised Gauß-Green formula* (see e.g. [AFP00, Theorem 3.36])

$$\begin{aligned} \int_A \operatorname{div} \varphi \, dx &= -\int_{\mathbb{R}^n} \langle \varphi, \nu_A \rangle \, d|D\mathbb{1}_A| \\ &= -\int_{\mathcal{F}A} \langle \varphi, \nu_A \rangle \, d\mathcal{H}^{n-1}, \qquad \varphi \in C_0^1(\mathbb{R}^n, \mathbb{R}^n), \end{aligned} \tag{1.12}$$

holds.

1.4 From the L^2-diffusion inequality to the isoperimetric inequality

Apart from being a nice consequence of the Riesz-Sobolev inequality, the L^2-diffusion inequality has interesting relations with the isoperimetric inequality. M. Ledoux [Led94] discovered that the L^2-diffusion inequality

$$\|T(t)\mathbb{1}_A\|_{L^2} \le \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t \ge 0, \tag{1.13}$$

implies the isoperimetric inequality.

Observe that we use the notation

$$\langle f, g \rangle = \int\limits_{\mathbb{R}^n} f(x) g(x)\, dx$$

not only for the inner product in $L^2(\mathbb{R}^n)$ but also for the dual pairing when $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, $\frac{1}{p} + \frac{1}{q} = 1$.
In particular we will look at the pairing $\langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c} \rangle$ which physically represents the amount of heat that has flowed out of A into the complement A^c after time t.

Using semigroup properties of $(T(t))_{t \geq 0}$ and further analysis for the explicit formula of the heat kernel one can prove that for every Caccioppoli set $A \subset \mathbb{R}^n$ this pairing satisfies the following estimate, see [Led94] and [Pre04].

Proposition 12. *Let $A \subset \mathbb{R}^n$ be a Caccioppoli set. Then*

$$\langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c} \rangle \leq \frac{\sqrt{t}}{\sqrt{\pi}} P(A) \tag{1.14}$$

holds for all $t \geq 0$.

Furthermore M. Ledoux proved that the bound (1.14) is optimal for a Euclidean ball as $t \to 0$:

Proposition 13. *For B a Euclidean ball in $\mathbb{R}^n$ it holds*

$$\lim_{t \searrow 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_B, \mathbb{1}_{B^c} \rangle = P(B). \tag{1.15}$$

Now the isoperimetric inequality can be deduced as follows: First, by the relation (see Section 1.1)

$$\|T(\tfrac{t}{2})\mathbb{1}_A\|_{L^2}^2 = \langle T(t)\mathbb{1}_A, \mathbb{1}_A \rangle_{L^2}$$

we rewrite the L^2-inequality (1.13) as

$$\langle T(t)\mathbb{1}_A, \mathbb{1}_A \rangle \leq \langle T(t)\mathbb{1}_B, \mathbb{1}_B \rangle, \qquad t \geq 0. \tag{1.16}$$

Using the elementary relations

$$\begin{aligned} |A| = \langle T(t)\mathbb{1}_A, \mathbb{1}_{\mathbb{R}^n} \rangle &= \langle T(t)\mathbb{1}_A, \mathbb{1}_A \rangle + \langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c} \rangle, \qquad t \geq 0, \\ |B| = \langle T(t)\mathbb{1}_B, \mathbb{1}_{\mathbb{R}^n} \rangle &= \langle T(t)\mathbb{1}_B, \mathbb{1}_B \rangle + \langle T(t)\mathbb{1}_B, \mathbb{1}_{B^c} \rangle, \qquad t \geq 0 \end{aligned}$$

and the fact that A and B have the same volume, it follows that (1.16) is equivalent to

$$\langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c} \rangle \geq \langle T(t)\mathbb{1}_B, \mathbb{1}_{B^c} \rangle, \qquad t \geq 0.$$

So with Propositions 12 and 13 we obtain that

$$P(A) \geq \lim_{t \searrow 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c} \rangle \geq \lim_{t \searrow 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_B, \mathbb{1}_{B^c} \rangle = P(B),$$

i.e.,

$$P(A) \geq P(B),$$

which is the isoperimetric inequality for Caccioppoli sets in $\mathbb{R}^n$.

1.5 Geometry of hypersurfaces in $\mathbb{R}^n$

We briefly introduce some notation from the theory of smooth hypersurfaces in $\mathbb{R}^n$, needed to describe the asymptotic expansions of the evolution of level sets in the next chapter.
We first recall some general facts about the metric, second fundamental form and mean curvature of hypersurfaces in $\mathbb{R}^n$ which are locally given as graphs. Then the corresponding formulas with respect to local normal coordinates will be given.

General notations

Let $\Sigma \subset \mathbb{R}^n$ be a smooth hypersurface. For every parametrisation $F : \mathbb{R}^{n-1} \supset U \to \Sigma$ of Σ a natural basis of the tangent space $T_p\Sigma$ at $p = F(x)$ is given by the set of the $n-1$ tangent vectors

$$\frac{\partial F}{\partial x_1}(x), ..., \frac{\partial F}{\partial x_{n-1}}(x).$$

Recall that locally we can always represent Σ as graph of a smooth function, i.e., for every $p \in \Sigma$ we find an open set $\Omega \subset \mathbb{R}^{n-1}$ and a smooth function $u : \Omega \to \mathbb{R}$ such that $F(x) = (x, u(x))$ is a local parametrisation of Σ. In this representation the basis vectors $\{\frac{\partial F}{\partial x_i}\}_{1\le i\le n-1}$ at $p = (x, u(x)) \in \Sigma$ take the form

$$\frac{\partial F}{\partial x_i}(x) = (0, ..., 0, \overset{(i)}{1}, 0, ..., D_i u(x)).$$

Hence the coefficients g_{ij} of the induced *metric* g with respect to $\{\frac{\partial F}{\partial x_i}\}_{1\le i\le n-1}$ are given by

$$\begin{aligned} g_{ij} = \left\langle \frac{\partial F}{\partial x_i}(x), \frac{\partial F}{\partial x_j}(x) \right\rangle_{\mathbb{R}^n} &= \left\langle (0, ..., 0, \overset{(i)}{1}, 0, ..., D_i u(x)), (0, ..., 0, \overset{(j)}{1}, 0, ..., D_j u(x)) \right\rangle_{\mathbb{R}^n} \\ &= \delta_{ij} + D_i u(x) \cdot D_j u(x), \qquad 1 \le i, j \le n-1, \quad (1.17) \end{aligned}$$

where $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ denotes the standard scalar product in $\mathbb{R}^n$.

A unit normal vector ν at $p = (x, u(x))$ is given by

$$\nu(p) = \frac{(-Du(x), 1)}{\sqrt{1 + |Du(x)|^2}}$$

and its differential $D\nu(p)$, the *Weingarten operator*, is a self-adjoint linear map on $T_p\Sigma$ with respect to the metric g. Its $n-1$ real eigenvalues $\lambda_1, ..., \lambda_{n-1}$ are called *principal curvatures* of Σ at p, and the corresponding eigenvectors are the *principal curvature directions.*

Given the metric g and the Weingarten operator $D\nu$ at $p \in \Sigma$ we define by

$$A(X, Y) := \langle D\nu(p)X, Y \rangle_g, \qquad X, Y \in T_p\Sigma$$

the *second fundamental form* A which, by the self-adjointness of $D\nu$, is a bilinear symmetric form on $T_p\Sigma$.

We denote by h_{ij} the coefficients of A. With respect to the basis $\{\frac{\partial F}{\partial x_i}\}_{1\leq i\leq n-1}$ of $T_p\Sigma$ they are given by

$$h_{ij} = A\Big(\frac{\partial F}{\partial x_i}(x), \frac{\partial F}{\partial x_j}(x)\Big),$$

and, in case Σ is parametrised as graph of a smooth function u, we have

$$h_{ij} = \frac{-D_iD_ju}{\sqrt{1+|Du|^2}}. \tag{1.18}$$

The trace of the Weingarten operator $D\nu$ at p, i.e., the sum of the principal curvatures $\lambda_1 + \lambda_2 + ... + \lambda_{n-1}$, is the *mean curvature* H of Σ at p. In terms of the metric g and the second fundamental form A it can be expressed as $H = \sum\limits_{ij} g^{ij}h_{ij} = \sum\limits_{i} h^i_i$.

We further denote by $|A|^2$ the squared norm of A. In terms of the coefficients h_{ij} it becomes $|A|^2 = \sum\limits_{ijkl} g^{ij}g^{kl}h_{ik}h_{jl} = \sum\limits_{il} h^l_i\, h^i_l$ and in terms of the principle curvatures $|A|^2 = \lambda_1^2 + \lambda_2^2 + ... + \lambda_{n-1}^2$.

In the following we will also need the quantity $\operatorname{tr} A^3$, the trace of the third power of A. It can be expressed as $\operatorname{tr} A^3 = \sum\limits_{ijk} h^j_i\, h^k_j\, h^i_k$ and in terms of the principal curvatures as $\operatorname{tr} A^3 = \lambda_1^3 + \lambda_2^3 + ... + \lambda_{n-1}^3$.

Finally, the *Christoffel symbols* of the metric g_{ij} are given by

$$\Gamma^k_{ij} \;=\; \frac{1}{2}\sum_l g^{kl}\Big(\frac{\partial}{\partial x_i}g_{jl} + \frac{\partial}{\partial x_j}g_{il} - \frac{\partial}{\partial x_l}g_{ij}\Big). \tag{1.19}$$

Normal coordinate systems and geometry of ∂D

Let $D \subset \mathbb{R}^n$ be a compact set with smooth boundary ∂D which is a smooth closed hypersurface in $\mathbb{R}^n$. We fix a point $p \in \partial D$. After translation and rotation of D in $\mathbb{R}^n$, we may assume that p coincides with the origin of $\mathbb{R}^n$ and the *outer* unit normal vector $\vec{\nu}(p)$ at ∂D in p is given by the n-th standard unit normal vector $e_n = (0, 0, ..., 1)$ of $\mathbb{R}^n$.
We call such a coordinate system a *local normal coordinate system* at p with respect to ∂D since in these coordinates the boundary ∂D can be represented locally around p as graph of a smooth function $u : U \subset \mathbb{R}^{n-1} \to \mathbb{R}$ satisfying (since $\mathbb{R}^{n-1} \times \{0\}$ coincides with the tangent plane $T_p(\partial D)$)

$$u(0) = 0 \qquad \text{and} \qquad Du(0) = 0. \tag{1.20}$$

Then it follows from (1.17) and (1.18) that with respect to these coordinates the coefficients of the metric $g = g_{ij}$ and of the second fundamental form $A = h_{ij}$ of ∂D at p are given by

$$g_{ij} = \delta_{ij} \qquad \text{and} \qquad h_{ij}(p) = -D_iD_ju(0).$$

So the coefficients h_{ij} are the negative of the components of the Hessian of u at 0. We can further determine the mean curvature H of ∂D at p as

$$H(p) = \sum_{i,j} \delta^{ij} h_{ij}(p) = -\sum_{i} D_i D_i u(0) = -\Delta u(0),$$

i.e., given by minus the Laplacian of the representation u of ∂D.

Further (1.17) and (1.20) at p imply

$$\frac{\partial}{\partial x_k} g_{ij} \;=\; D_k D_i u \cdot D_j u + D_i u \cdot D_k D_j u \;=\; 0. \tag{1.21}$$

In particular it holds $\Gamma_{ij}^k = 0$ at p.

Chapter 2

Diffusion of characteristic functions: Short time behaviour

In this chapter we study the short time behaviour of the flow $t \mapsto T(t)\mathbb{1}_D$ and of the maps

$$t \mapsto \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle \qquad \text{and} \qquad t \mapsto \|T(t)\mathbb{1}_D\|_{L^2},$$

respectively. In particular we pursue two main aims:

In the first part we present a detailed treatment of the short time evolution of the level sets of $t \mapsto T(t)\mathbb{1}_D$ and determine the pointwise asymptotic behaviour for this evolution: We show that for short times the evolution of the level sets admits an asymptotic expansion in powers of $t^{1/2}$. We determine the coefficients up to order t^2 in terms of geometric invariants of the boundary ∂D and give a general formula for the coefficients of higher order.
Related questions on level sets have been studied by [Eva93], [BMO94] and [Cha04]. In particular, the analytic techniques used in the proof of Proposition 18 and Theorem 19 go back to L.C. Evans [Eva93] who studied approximation of (nonlinear) mean curvature flow by (linear) heat flows starting from characteristic functions.

Our second aim is to generalise M. Ledoux's result (see Chapter 1, Proposition 13) by proving that the formula

$$\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = P(D) \tag{2.1}$$

holds for compact sets with smooth boundary and even for all Caccioppoli sets in $\mathbb{R}^n$.

We will treat this question from two different points of view: For a compact set $D \subset \mathbb{R}^n$ with smooth boundary we first apply the above results on the asymptotic expansion for the level sets to deduce (2.1).
The second approach, using methods from geometric measure theory, allows to prove (2.1) even for all Caccioppoli sets in $\mathbb{R}^n$, but gives less insight into the "geometric nature" of the flow.
This last result was obtained in collaboration with M. Miranda (jr), D. Pallara and F. Paronetto (see [MPPP05]) and the proof is based on the measure-theoretic properties of the reduced boundary $\mathcal{F}D$ of D.

2.1 Asymptotic expansion for the evolution of level sets

For a given compact set $D \subset \mathbb{R}^n$ with smooth boundary ∂D we now study the evolution of level sets in $\mathbb{R}^n$ induced by the heat flow $t \mapsto T(t)\mathbb{1}_D$. In other words, we treat the time dependent motion of subsets in $\mathbb{R}^n$ on which the function $T(t)\mathbb{1}_D : \mathbb{R}^n \to (0,1)$ takes a given value $\lambda \in (0,1)$. To be precise we define the following.

Definition 14. Given a compact set $D \subset \mathbb{R}^n$. For $\lambda \in (0,1)$ we call

$$t \mapsto D_\lambda(t) := \{x \in \mathbb{R}^n : T(t)\mathbb{1}_D(x) = \lambda\}$$

the *evolution of level sets induced by the heat flow* $t \mapsto T(t)\mathbb{1}_D$.

Physically this means that we consider the evolution of subsets in $\mathbb{R}^n$ of constant temperature $\lambda \in (0,1)$, when the initial heat distribution is given by the characteristic function $\mathbb{1}_D$. Note that, since the function $T(t)\mathbb{1}_D$ is smooth for every $t > 0$, by the implicit function theorem the level set $D_\lambda(t)$ will be a smooth hypersurface in $\mathbb{R}^n$ if λ is a regular value of $T(t)\mathbb{1}_D$, i.e., if $\nabla T(t)\mathbb{1}_D(x) \neq 0$ for every $x \in D_\lambda(t)$.

We need the following definition in order to understand how a given value of $\lambda \in (0,1)$, i.e., the height of the level, influences the motion of the level set $D_\lambda(t)$. We intuitively expect that the motion of level sets will depend on the local geometry of ∂D but also on the concrete choice of the level λ.

Definition 15. We define a *Gaussian error function* $\Phi : \mathbb{R} \to (0,1)$ by

$$\Phi(x) := \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{x} e^{\frac{-z^2}{4}} dz.$$

Since Φ is bijective, we denote its inverse by

$$c_\lambda := \Phi^{-1}(\lambda), \qquad \lambda \in (0,1),$$

i.e., c_λ is the unique real number such that

$$\frac{1}{\sqrt{4\pi}} \int_{-\infty}^{c_\lambda} e^{\frac{-z^2}{4}} dz = \lambda.$$

The function $z \mapsto e^{\frac{-z^2}{4}}$ has no elementary primitive function, thus no concrete formula for c_λ can be expected.

Remark 16. By the definition of Φ we have the following properties

$$\lim_{x \to -\infty} \Phi(x) = 0, \qquad \lim_{x \to \infty} \Phi(x) = 1, \qquad \Phi(0) = \frac{1}{2}.$$

In particular, it holds that

$$
\begin{aligned}
c_\lambda < 0 \quad &\text{if} \quad 0 < \lambda < \frac{1}{2}, \\
c_\lambda = 0 \quad &\text{if} \quad \lambda = \frac{1}{2}, \\
c_\lambda > 0 \quad &\text{if} \quad \frac{1}{2} < \lambda < 1.
\end{aligned}
$$

The most important tool to study the geometric evolution of $t \mapsto T(t)\mathbb{1}_D$ will be the *normal distance function* which we define as follows.

Definition 17. Given a compact set $D \subset \mathbb{R}^n$ with smooth boundary, a point $p \in \partial D$ and a level $\lambda \in (0, 1)$. We define $d_\lambda(t)$ to be the real valued function of t such that

$$p + d_\lambda(t) \cdot \vec{\nu}(p) \in D_\lambda(t),$$

i.e., $d_\lambda(t)$ gives the normal distance the level set $D_\lambda(t)$ has moved away from ∂D after time t. We call $d_\lambda(t)$ the *normal distance function* with respect to the level λ.

Note that, since for every $\lambda \in (0, 1)$ the level set $D_\lambda(t)$ will become empty after a certain time, $d_\lambda(t)$ is never defined on the whole of $(0, \infty)$. In particular, for λ close to 1, $d_\lambda(t)$ will be defined only for very short time intervals.

In order to illustrate the method how to obtain the asymptotic expansion for the normal distance function $d_\lambda(t)$ we start in the next subsection with the one-dimensional case and then proceed with the (more complicated) n-dimensional situation where the geometry of the boundary comes into play.

The one-dimensional case

Let $D \subset \mathbb{R}$ be a compact interval and denote by $t \mapsto T(t)\mathbb{1}_D$ the heat flow starting from its characteristic function $\mathbb{1}_D$. Here, the "normal" distance $d_\lambda(t)$ simply becomes the distance between the level set $D_\lambda(t)$ and the boundary ∂D.

We obtain the following result for its asymptotic behaviour as $t \to 0$.

Proposition 18 (Asymptotic behaviour of the distance; one-dimensional). *Let $D \subset \mathbb{R}$ be a compact interval. Then the distance function $d_\lambda(t)$ describing the evolution of level sets $D_\lambda(t)$ for a given level $\lambda \in (0, 1)$ has the following asymptotic behaviour*

$$d_\lambda(t) = -c_\lambda t^{1/2} + O(e^{-\alpha/t}) \qquad \text{as } t \to 0. \tag{2.2}$$

Proof: By translation invariance of heat diffusion we may assume that $D = [-a, 0]$ for some $a > 0$. We take $x = d_\lambda(t)$ and consider

$$\lambda = T(t)\mathbb{1}_D(x) = T(t)\mathbb{1}_D(d_\lambda(t)).$$

The integral representation of $T(t)\mathbb{1}_D(x)$ then yields

$$\lambda = \frac{1}{\sqrt{4\pi t}} \int_D e^{\frac{-|y-d_\lambda(t)|^2}{4t}}\, dy = \frac{1}{\sqrt{4\pi t}} \int_{-a}^{0} e^{\frac{-|y-d_\lambda(t)|^2}{4t}}\, dy.$$

In order to eliminate the t-dependence in the exponential function, we change variables by setting $z := \frac{y-d_\lambda(t)}{t^{1/2}}$ and obtain

$$\lambda = \frac{1}{2\sqrt{\pi}} \int_{-\frac{a+d_\lambda(t)}{t^{1/2}}}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}}\, dz.$$

Now, since

$$\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz = \underbrace{\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{-\frac{a+d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz}_{=O(e^{-\alpha/t})} + \underbrace{\frac{1}{2\sqrt{\pi}} \int_{-\frac{a+d_\lambda(t)}{t^{1/2}}}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz}_{=\lambda},$$

(where the first integral on the right hand side tends exponentially to zero since $-\frac{a+d_\lambda(t)}{t^{1/2}} \to -\infty$ sufficiently fast as $t \to 0$), it holds that

$$\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz = \lambda + O(e^{-\alpha/t}). \tag{2.3}$$

We choose $c_\lambda = \Phi^{-1}(\lambda)$ (cf. Definition 15) such that

$$\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{c_\lambda} e^{\frac{-z^2}{4}} dz = \lambda$$

and rewrite (2.3) as

$$\begin{aligned} \lambda &= \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{c_\lambda} e^{\frac{-z^2}{4}} dz + \frac{1}{2\sqrt{\pi}} \int_{c_\lambda}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz + O(e^{-\alpha/t}) \\ &= \lambda + \frac{1}{2\sqrt{\pi}} \int_{c_\lambda}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz + O(e^{-\alpha/t}). \end{aligned}$$

After subtracting λ on both sides and omitting the constant $\frac{1}{2\sqrt{\pi}}$ we obtain

$$\int_{c_\lambda}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz = O(e^{-\alpha/t}), \tag{2.4}$$

which will be crucial in order to determine the asymptotic behaviour of $d_\lambda(t)$ as $t \to 0$. Since $e^{\frac{-z^2}{4}}$ is strictly positive, (2.4) implies that the length of the integration interval has to go to zero. To conclude the proof it only remains to show that the convergence is exponentially fast.
Since we are interested in the asymptotic behaviour as $t \to 0$, we fix a small time $t_0 > 0$ and determine a lower bound for the integral (2.4). Therefore we denote its integration interval by

$$I(t) := [c_\lambda, \frac{-d_\lambda(t)}{t^{1/2}}]$$

and its length by

$$|I(t)| := \frac{-d_\lambda(t)}{t^{1/2}} - c_\lambda.$$

We further set

$$K := \min_{0<t<t_0} \{e^{\frac{-z^2}{4}} : z \in I(t)\}.$$

Since the lengths of the intervals $I(t)$ are uniformly bounded from above for $0 < t < t_0$, the exponential function can not get arbitrarily close to zero. Therefore K is strictly positive.

We now take the product of K and the length $|I(t)|$ of the integration interval and obtain a lower bound for (2.4)

$$0 < K \cdot |I(t)| < \int_{c_\lambda}^{\frac{-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z^2}{4}} dz, \qquad 0 < t < t_0,$$

which implies

$$|I(t)| = O(e^{-\alpha/t}).$$

Therefore

$$\frac{-d_\lambda(t)}{t^{1/2}} - c_\lambda = O(e^{-\alpha/t}),$$

i.e.,

$$d_\lambda(t) = -c_\lambda t^{1/2} + O(e^{-\alpha/t}).$$

□

We now come to the n-dimensional situation.

The n-dimensional case

We take $D \subset \mathbb{R}^n$ to be a compact set with smooth boundary. Our main theorem on the asymptotic expansion of the evolution of the level sets $D_\lambda(t)$ is the following. The proof will be given successively in the next sections.

Theorem 19 (Asymptotic behaviour of the normal distance; n-dimensional). *The normal distance function $d_\lambda(t)$ describing the evolution of the level sets $D_\lambda(t)$ for a given level $\lambda \in (0,1)$ admits an asymptotic expansion in powers of $t^{1/2}$*

$$d_\lambda(t) = a_{1/2}t^{1/2} + a_1 t + a_{3/2}t^{3/2} + a_2 t^2 + ... + a_k t^k + O(t^{k+1}) \qquad \text{as } t \to 0. \qquad (2.5)$$

The first five coefficients can be computed explicitly as

$$\begin{aligned} a_{1/2} &= -c_\lambda, \\ a_1 &= \Delta u = -H, \\ a_{3/2} &= 0, \\ a_2 &= \frac{1}{2}\Delta^2 u = -\frac{1}{2}(\triangle_{\partial D} H + H|A|^2 + 2\,\mathrm{tr}\, A^3), \\ a_{5/2} &= 0, \end{aligned}$$

i.e., the normal distance between ∂D and $D_\lambda(t)$ behaves asymptotically as

$$d_\lambda(t) = -t^{1/2}c_\lambda - tH - \frac{t^2}{2}(\triangle_{\partial D}H + H|A|^2 + 2\operatorname{tr}A^3) + O(t^3) \qquad \textit{as } t \to 0.$$

Remark 20. (i) Note that in the expansion of $d_\lambda(t)$ we have a strict separation between the height of the level λ and geometric quantities of ∂D: The asymptotic behaviour in order $t^{1/2}$ is completely independent of the geometry of ∂D, whereas the behaviour of $d_\lambda(t)$ in higher orders is independent of λ and only depends on the geometry of ∂D.

(ii) Since the leading coefficient in the expansion is given by $-c_\lambda$ and geometric quantities occur first in order t, we see that the short time evolution of the level sets $D_\lambda(t)$ is (in the lowest order $t^{1/2}$) governed by the value of λ. Since $-c_\lambda$ is positive if $\lambda \in (0, \frac{1}{2})$ and negative if $\lambda \in (\frac{1}{2}, 1)$, we obtain that for short times the evolution of the level sets $D_\lambda(t)$ is directed to the complement of D if $\lambda \in (0, \frac{1}{2})$ and to the interior of D if $\lambda \in (\frac{1}{2}, 1)$, as one would expect intuitively.

(iii) The expansion gives a deep insight into the geometric nature of heat flows starting from characteristic functions: The coefficient $-c_\lambda$ in order $t^{1/2}$ is responsible for the "rough" diffusion of the heat contained in D without recognizing the geometry of ∂D. Simultanously with the coefficient $-H$ in order t the heat equation immediately optimizes the "shape" of the level sets $D_\lambda(t)$ since the flow of a closed surface in outer normal direction by minus its mean curvature (the classical *mean curvature flow*) is the gradient flow for the area functional, i.e., it is the optimal geometric flow in order to minimize the surface area. So, for short times, apart from only diffusing the heat from D into D^c through the boundary ∂D, the heat semigroup does this in a physically optimal way.

(iv) From the coefficients c_λ we also recover the infinite speed of propagation of heat diffusion: For small $t > 0$ and every positive distance d we find a (maybe very low) level λ such that the level set $D_\lambda(t)$ has distance from ∂D greater than d.

Proof: Given a fixed point $p \in \partial D$. According to Chapter 1, Section 1.5 we take a normal coordinate system at $p \in \partial D$ such that $p = 0$ and $\vec{\nu}(p) = (0, 0, ..., 1)$. Let $Q := Q_{\mathbb{R}^n} = \{x \in \mathbb{R}^n : |x_i| \le 1, i = 1, ..., n\}$ be the unit cube in $\mathbb{R}^n$ and $\tilde{Q} := Q_{\mathbb{R}^{n-1}}$ the corresponding unit cube in $\mathbb{R}^{n-1}$.
We assume that within the unit cube Q the boundary ∂D is represented by the graph of a smooth function $\tilde{u} : \tilde{Q} \subset \mathbb{R}^{n-1} \to \mathbb{R}$ such that $|\tilde{u}(\tilde{y})| < 1$ for $\tilde{y} \in \tilde{Q}$. For technical reasons we extend $\tilde{u}$ from $\tilde{Q}$ to a bounded smooth function $u : \mathbb{R}^{n-1} \to \mathbb{R}$ on the whole of $\mathbb{R}^{n-1}$.

We take $x = (0, 0, ..., d_\lambda(t))$ and consider

$$\lambda = T(t)\mathbb{1}_D(x) = T(t)\mathbb{1}_D(0, 0, ..., d_\lambda(t)).$$

The integral representation of $T(t)\mathbb{1}_D(x)$ then yields

$$\lambda = \frac{1}{(4\pi t)^{n/2}} \int_D e^{\frac{-|y-(0,0,...,d_\lambda(t))|^2}{4t}}\, dy = \frac{1}{(4\pi t)^{n/2}} \int_D e^{\frac{-|\tilde{y}|^2 - (y_n - d_\lambda(t))^2}{4t}}\, dy.$$

We reduce our consideration to the unit cube Q around $p = 0$ since the short time influence coming from outside Q will become exponentially small as $t \to 0$, i.e.,

$$\begin{aligned}\lambda &= \frac{1}{(4\pi t)^{n/2}} \int_{D\cap Q} e^{\frac{-|\tilde{y}|^2-(y_n-d_\lambda(t))^2}{4t}}\, dy + \frac{1}{(4\pi t)^{n/2}} \int_{D\setminus Q} e^{\frac{-|\tilde{y}|^2-(y_n-d_\lambda(t))^2}{4t}}\, dy \\ &= \frac{1}{(4\pi t)^{n/2}} \int_{\tilde{Q}} \int_{-1}^{u(\tilde{y})} e^{\frac{-|\tilde{y}|^2-(y_n-d_\lambda(t))^2}{4t}}\, dy_n d\tilde{y} + O(e^{-\alpha/t})\end{aligned}$$

for some $\alpha > 0$. Now, in order to eliminate the t-dependence in the exponential function, we change variables by setting $(\tilde{z}, z_n) := (\frac{\tilde{y}}{t^{1/2}}, \frac{y_n - d_\lambda(t)}{t^{1/2}})$ and obtain

$$\begin{aligned}\lambda &= \frac{1}{(4\pi)^{n/2}} \int_{\frac{\tilde{Q}}{t^{1/2}}} \int_{-\frac{1+d_\lambda(t)}{t^{1/2}}}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2-z_n^2}{4}}\, dz_n d\tilde{z} + O(e^{-\alpha/t}) \\ &= \frac{1}{(4\pi)^{n/2}} \int_{\frac{\tilde{Q}}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\frac{1+d_\lambda(t)}{t^{1/2}}}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}}\, dz_n d\tilde{z} + O(e^{-\alpha/t}).\end{aligned}$$

Now, since

$$\begin{aligned}&\frac{1}{(4\pi)^{n/2}} \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\infty}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} \\ &= \frac{1}{(4\pi)^{n/2}} \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \Big(\int_{-\infty}^{-\frac{1+d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n + \int_{-\frac{1+d_\lambda(t)}{t^{1/2}}}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n \Big) d\tilde{z} \\ &= \left.\frac{1}{(4\pi)^{n/2}} \int_{\frac{\tilde{Q}}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\frac{1+d_\lambda(t)}{t^{1/2}}}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} \right\} = \lambda + O(e^{-\alpha/t}) \\ &\left.\begin{aligned} &+ \frac{1}{(4\pi)^{n/2}} \int_{\mathbb{R}^{n-1}\setminus\frac{\tilde{Q}}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\frac{1+d_\lambda(t)}{t^{1/2}}}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} \\ &+ \frac{1}{(4\pi)^{n/2}} \int_{\frac{\tilde{Q}}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\infty}^{-\frac{1+d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} \\ &+ \frac{1}{(4\pi)^{n/2}} \int_{\mathbb{R}^{n-1}\setminus\frac{\tilde{Q}}{t^{1/2}}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\infty}^{-\frac{1+d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} \end{aligned}\right\} = O(e^{-\alpha/t})\end{aligned}$$

(where the last three summands tend exponentially to zero since $\mathbb{R}^{n-1} \setminus \frac{\tilde{Q}}{t^{1/2}} \to \emptyset$ and $-\frac{1+d_\lambda(t)}{t^{1/2}} \to -\infty$ sufficiently fast as $t \to 0$), it holds that

$$\lambda = \frac{1}{(4\pi)^{n/2}} \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{-\infty}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} dz_n d\tilde{z} + O(e^{-\alpha/t}). \tag{2.6}$$

We now choose $c_\lambda = \Phi^{-1}(\lambda)$ (cf. Definition 15) and, by factorisation, obtain

$$\begin{aligned}\frac{1}{(4\pi)^{n/2}}\int_{\mathbb{R}^{n-1}}\int_{-\infty}^{c_\lambda} e^{\frac{-|z|^2}{4}}dz &= \frac{1}{(4\pi)^{n/2}}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\int_{-\infty}^{c_\lambda} e^{\frac{-z_n^2}{4}}dz_n d\tilde{z}\\ &= \underbrace{\frac{1}{(4\pi)^{(n-1)/2}}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}d\tilde{z}}_{=1}\cdot\underbrace{\frac{1}{(4\pi)^{1/2}}\int_{-\infty}^{c_\lambda} e^{\frac{-z_n^2}{4}}dz_n}_{=\lambda}\\ &= \lambda.\end{aligned}$$

Using this identity we write (2.6) as

$$\begin{aligned}\lambda &= \frac{1}{(4\pi)^{n/2}}\int_{\mathbb{R}^{n-1}}\int_{-\infty}^{c_\lambda} e^{\frac{-|z|^2}{4}}dz + \frac{1}{(4\pi)^{n/2}}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\int_{c_\lambda}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}}dz_n d\tilde{z} + O(e^{-\alpha/t})\\ &= \lambda + \frac{1}{(4\pi)^{n/2}}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\int_{c_\lambda}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}}dz_n d\tilde{z} + O(e^{-\alpha/t}),\end{aligned}$$

and by subtracting λ on both sides we obtain the relation

$$\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\underbrace{\int_{c_\lambda}^{\frac{u(t^{1/2}\tilde{z})-d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}}dz_n}_{=:B_t(\tilde{z})} d\tilde{z} = O(e^{-\alpha/t}), \tag{2.7}$$

which will be essential to obtain a determining equation for the normal distance $d_\lambda(t)$. Since we are interested in the asymptotic behaviour of $d_\lambda(t)$ as $t \to 0$, we fix some small $t_0 > 0$ and determine a lower bound for the integral $B_t(\tilde{z})$ that is valid for all $0 < t < t_0$. We set

$$I(t,\tilde{z}) := [c_\lambda, \frac{u(t^{1/2}\tilde{z}) - d_\lambda(t)}{t^{1/2}}]$$

for the integration interval and denote its length by

$$|I(t,\tilde{z})| := \frac{u(t^{1/2}\tilde{z}) - d_\lambda(t)}{t^{1/2}} - c_\lambda.$$

Since $e^{\frac{-|\tilde{z}|^2}{4}}$ is strictly positive, it follows that $B_t(\tilde{z})$ has to go to zero for every $\tilde{z} \in \mathbb{R}^{n-1}$ as $t \to 0$, which further implies by the strict positivity of $e^{\frac{-z_n^2}{4}}$ that also $|I(t,\tilde{z})| \to 0$ as $t \to 0$.
Since $u : \mathbb{R}^{n-1} \to \mathbb{R}$ is bounded by construction (see above), also $u(t^{1/2}\tilde{z})$ remains a bounded function of $\tilde{z}$ for every choice of $0 < t < t_0$, i.e., there exists a constant M such that

$$u(t^{1/2}\tilde{z}) \le M \qquad \text{for every } \tilde{z} \in \mathbb{R}^{n-1}, 0 < t < t_0,$$

which implies that the lengths of the intervals $I(t,\tilde{z})$ are uniformly bounded from above for $0 < t < t_0, \tilde{z} \in \mathbb{R}^{n-1}$. Further we set

$$K := \min_{0<t<t_0,\, \tilde{z}\in\mathbb{R}^{n-1}}\{e^{\frac{-z_n^2}{4}} : z_n \in I(t,\tilde{z})\}$$

being the uniform minimum of the integrand $e^{\frac{-z_n^2}{4}}$ on $I(t, \tilde{z})$ for every $0 < t < t_0$ and $\tilde{z} \in \mathbb{R}^{n-1}$, i.e.,

$$K \leq e^{\frac{-z_n^2}{4}} \qquad \text{for } z_n \in I(t, \tilde{z}) \text{ with } 0 < t < t_0 \text{ and } \tilde{z} \in \mathbb{R}^{n-1}.$$

Since the lengths of the intervals $I(t, \tilde{z})$ are uniformly bounded from above for $0 < t < t_0, \tilde{z} \in \mathbb{R}^{n-1}$ and the exponential function is strictly positive, also K is strictly positive.

We now take the product of K and the length $|I(t, \tilde{z})|$ of the integration interval to obtain the following lower bound for the integral $B_t(\tilde{z})$

$$0 \leq K \cdot |I(t, \tilde{z})| \leq B_t(\tilde{z}), \qquad \tilde{z} \in \mathbb{R}^{n-1}, 0 < t < t_0.$$

Since also $e^{\frac{-|\tilde{z}|^2}{4}}$ is strictly positive on $\mathbb{R}^{n-1}$, we conclude that

$$\begin{aligned} 0 &\leq K \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \cdot |I(t, \tilde{z})| \, d\tilde{z} \\ &= \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \cdot K \cdot |I(t, \tilde{z})| \, d\tilde{z} \\ &\leq \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \int_{c_\lambda}^{\frac{u(t^{1/2}\tilde{z}) - d_\lambda(t)}{t^{1/2}}} e^{\frac{-z_n^2}{4}} \, dz_n d\tilde{z} \qquad \text{for all } 0 < t \leq t_0. \end{aligned}$$

Omitting the constant K we by (2.7) obtain

$$\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \underbrace{\left(t^{-1/2}[u(t^{1/2}\tilde{z}) - d_\lambda(t) - t^{1/2}c_\lambda]\right)}_{=|I(t,\tilde{z})|} d\tilde{z} = O(e^{-\alpha/t}). \tag{2.8}$$

Using the Taylor expansion of $u(t^{1/2}\tilde{z})$ in $\tilde{z} = 0$ and the fact that u satisfies $u(0) = 0$ and $Du(0) = 0$ we have

$$\begin{aligned} u(t^{1/2}\tilde{z}) &= \underbrace{u(0)}_{=0} + \underbrace{t^{1/2}u_i(0)z_i}_{=0} + \frac{t}{2}u_{ij}(0)z_iz_j + \frac{t^{3/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t^2}{24}u_{ijkr}(0)z_iz_jz_kz_r + O(t^{5/2}|\tilde{z}|^5) \\ &= \frac{t}{2}u_{ij}(0)z_iz_j + \frac{t^{3/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t^2}{24}u_{ijkr}(0)z_iz_jz_kz_r + O(t^{5/2}|\tilde{z}|^5), \end{aligned}$$

where we have used the convention that we always sum up over repeated indices, e.g., $u_{ijk}(0)z_iz_jz_k$ means $\sum_{i,j,k}^{n-1} u_{ijk}(0)z_iz_jz_k$.

So we write $|I(t, \tilde{z})|$ as

$$\begin{aligned} |I(t, \tilde{z})| &= t^{-1/2}[u(t^{1/2}\tilde{z}) - d_\lambda(t) - t^{1/2}c_\lambda] \\ &= t^{-1/2}\Big[\frac{t}{2}u_{ij}(0)z_iz_j + \frac{t^{3/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t^2}{24}u_{ijkr}(0)z_iz_jz_kz_r - d_\lambda(t) - t^{1/2}c_\lambda + O(t^{5/2}|\tilde{z}|^5)\Big] \\ &= \underbrace{t^{1/2}\Big[\frac{1}{2}u_{ij}(0)z_iz_j + \frac{t^{1/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t}{24}u_{ijkr}(0)z_iz_jz_kz_r - \frac{d_\lambda(t)}{t} - \frac{c_\lambda}{t^{1/2}}\Big] + O(t^2|\tilde{z}|^5)}_{=a}. \end{aligned}$$

Then we replace $|I(t,\tilde z)|$ by a in (2.8) and obtain that

$$\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} \underbrace{t^{1/2}\Big[\frac{1}{2}u_{ij}(0)z_iz_j + \frac{t^{1/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t}{24}u_{ijkr}(0)z_iz_jz_kz_r - \frac{d_\lambda(t)}{t} - \frac{c_\lambda}{t^{1/2}}\Big] + O(t^2|\tilde z|^5)}_{=a}\, d\tilde z$$
$$= O(e^{-\alpha/t}).$$

Comparing $O(t^2|\tilde z|^5)$ and $O(e^{-\alpha/t})$ yields

$$t^{1/2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} \Big[\frac{1}{2}u_{ij}(0)z_iz_j + \frac{t^{1/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t}{24}u_{ijkr}(0)z_iz_jz_kz_r - \frac{d_\lambda(t)}{t} - \frac{c_\lambda}{t^{1/2}}\Big] d\tilde z = O(t^2)$$

and therefore

$$\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} \Big[\frac{1}{2}u_{ij}(0)z_iz_j + \frac{t^{1/2}}{6}u_{ijk}(0)z_iz_jz_k + \frac{t}{24}u_{ijkr}(0)z_iz_jz_kz_r - \frac{d_\lambda(t)}{t} - \frac{c_\lambda}{t^{1/2}}\Big] d\tilde z = O(t^{3/2}).$$

We add another summand in the Taylor expansion of u and so we have that

$$\begin{aligned}
&\frac{1}{2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ij}(0)z_iz_j\, d\tilde z + \underbrace{\frac{t^{1/2}}{6}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ijk}(0)z_iz_jz_k\, d\tilde z}_{=0} \\
&+\frac{t}{24}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ijkr}(0)z_iz_jz_kz_r\, d\tilde z + \underbrace{\frac{t^{3/2}}{120}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ijkrm}(0)z_iz_jz_kz_rz_m\, d\tilde z}_{=0} \\
&-\Big(\frac{d_\lambda(t)}{t} + \frac{c_\lambda}{t^{1/2}}\Big)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z \;=\; O(t^2),
\end{aligned} \tag{2.9}$$

where the summands with the parentheses vanish by the symmetry of Gaussian integrals (see also Proposition 21). Further, we will show below (Corollary 23) that

$$\frac{1}{2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ij}(0)z_iz_j\, d\tilde z = \Delta u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z \tag{2.10}$$

and (Proposition 24) that

$$\frac{1}{24}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} u_{ijkr}(0)z_iz_jz_kz_r\, d\tilde z = \frac{1}{2}\Delta^2 u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z. \tag{2.11}$$

So this finally yields

$$\Delta u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z + t\cdot\frac{1}{2}\Delta^2 u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z - \Big(\frac{d_\lambda(t)}{t} + \frac{c_\lambda}{t^{1/2}}\Big)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z = O(t^2),$$

hence

$$\Big(\Delta u(0) + t\cdot\frac{1}{2}\Delta^2 u(0) - \frac{d_\lambda(t)}{t} - \frac{c_\lambda}{t^{1/2}}\Big)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}} d\tilde z = O(t^2).$$

By $\Delta u(0) = -H$ we obtain an explicit expression for $\frac{d_\lambda(t)}{t}$ as

$$\frac{d_\lambda(t)}{t} = -\frac{c_\lambda}{t^{1/2}} - H + t\cdot\frac{1}{2}\Delta^2 u(0) + O(t^2),$$

and therefore

$$d_\lambda(t) = -c_\lambda t^{1/2} - t \cdot H + t^2 \cdot \frac{1}{2}\Delta^2 u(0) + O(t^3).$$

It remains to prove the equalities (2.10) and (2.11) and the fact that $\frac{1}{2}\Delta^2 u(0) = -\frac{1}{2}(\triangle_{\partial D} H + H|A|^2 + 2\,\mathrm{tr}\,A^3)$ which we will do in the next section. $\square$

2.1.1 The coefficients a_1 and a_2

We first show the identities

$$\frac{1}{2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} u_{ij}(0)\, z_i z_j \, d\tilde{z} = \Delta u(0) \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z}$$

and

$$\frac{1}{24}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} u_{ijkr}(0)\, z_i z_j z_k z_r \, d\tilde{z} = \frac{1}{2}\Delta^2 u(0) \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z},$$

which we have used at the end (2.10), (2.11) of the above proof. For this purpose we start with an interesting observation on the symmetry of Gaussian integrals.

Proposition 21. *For $p \in \mathbb{N}$ we have*

$$\int_{\mathbb{R}} x^p\, e^{\frac{-x^2}{4}}\, dx = \begin{cases} \frac{p!}{(\frac{p}{2})!} \int_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx, & p \text{ even}, \\ 0, & p \text{ odd}. \end{cases}$$

And generally, for $p_1, ..., p_n \in \mathbb{N}$,

$$\int_{\mathbb{R}^n} x_1^{p_1} x_2^{p_2} ... x_n^{p_n}\, e^{\frac{-|x|^2}{4}}\, dx = \begin{cases} \left(\prod_{i=1}^{n} \frac{p_i!}{(\frac{p_i}{2})!}\right) \int_{\mathbb{R}^n} e^{\frac{-|x|^2}{4}}\, dx, & p_1, ..., p_n \text{ all even}, \\ 0, & \text{one of the } p_i \text{ is odd}. \end{cases}$$

Proof: Let $p \in \mathbb{N}$ be even, i.e., $p = 2q$ for some $q \in \mathbb{N}$. Then, in one dimension we have for arbitrary $a > 0$ (see e.g. [GR65, 3.461.2]) that

$$\int_{\mathbb{R}} x^p\, e^{-ax^2}\, dx = \int_{\mathbb{R}} x^{2q}\, e^{-ax^2}\, dx = \frac{1 \cdot 3 \cdot ... \cdot (2q-1)}{2^{q+1} a^{q+\frac{1}{2}}} \cdot 2\sqrt{\pi}.$$

We take $a = \frac{1}{4}$, use the fact that $\int_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx = 2\sqrt{\pi}$ and obtain

$$\begin{aligned} \int_{\mathbb{R}} x^{2q} e^{\frac{-x^2}{4}}\, dx &= \frac{1 \cdot 3 \cdot ... \cdot (2q-1)}{2^{q+1}\, (\frac{1}{4})^{q+\frac{1}{2}}} \int_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx \\ &= 1 \cdot 3 \cdot ... \cdot (2q-1) \cdot 2^q \int_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx. \end{aligned}$$

By the elementary fact that

$$\begin{aligned}\frac{(2q)!}{q!} &= \frac{1\cdot 2\cdot 3\cdot 4\cdot ...\cdot 2q}{1\cdot 2\cdot ...\cdot q}\\ &= 1\cdot\frac{2}{1}\cdot 3\cdot\frac{4}{2}\cdot ...\cdot\frac{2q-2}{q-2}\cdot(2q-1)\cdot\frac{2q}{q}\\ &= 1\cdot 2\cdot 3\cdot 2\cdot ...\cdot 2\cdot(2q-1)\cdot 2\\ &= 1\cdot 3\cdot ...\cdot(2q-1)\cdot 2^q\end{aligned}$$

we conclude

$$\int\limits_{\mathbb{R}} x^p\, e^{\frac{-x^2}{4}}\, dx = \int\limits_{\mathbb{R}} x^{2q} e^{\frac{-x^2}{4}}\, dx = \frac{(2q)!}{q!}\int\limits_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx = \frac{p!}{(\frac{p}{2})!}\int\limits_{\mathbb{R}} e^{\frac{-x^2}{4}}\, dx.$$

In case $p\in\mathbb{N}$ is odd, the integrand $x^p e^{\frac{-x^2}{4}}$ is anti-symmetric with respect to the origin, so

$$\int\limits_{\mathbb{R}} x^p e^{\frac{-x^2}{4}}\, dx = 0.$$

If all the exponents $p_1, ..., p_n$ are even, the general n-dimensional case follows by factorisation

$$\begin{aligned}\int\limits_{\mathbb{R}^n} x_1^{p_1} x_2^{p_2} ... x_n^{p_n} e^{\frac{-|x|^2}{4}}\, dx &= \int\limits_{\mathbb{R}} x_1^{p_1} e^{\frac{-x_1^2}{4}}\, dx_1\cdot ...\cdot\int\limits_{\mathbb{R}} x_n^{p_n} e^{\frac{-x_n^2}{4}}\, dx_n\\ &= \frac{p_1!}{(\frac{p_1}{2})!}\int\limits_{\mathbb{R}} e^{\frac{-x_1^2}{4}}\, dx_1\cdot ...\cdot\frac{p_n!}{(\frac{p_n}{2})!}\int\limits_{\mathbb{R}} e^{\frac{-x_n^2}{4}}\, dx_n\\ &= \Big(\prod_{i=1}^n \frac{p_i!}{(\frac{p_i}{2})!}\Big)\int\limits_{\mathbb{R}^n} e^{\frac{-|x|^2}{4}}\, dx.\end{aligned}$$

In case one p_i is odd, the factor containing this p_i and therefore the entire product is zero. □

In particular we obtain the following special cases.

Corollary 22. *It holds that*

$$\int_{\mathbb{R}^n} x_i x_j\, e^{\frac{-|x|^2}{4}}\, dx = \begin{cases} 2\int\limits_{\mathbb{R}^n} e^{\frac{-|x|^2}{4}} dx, & i=j,\\ 0, & i\neq j,\end{cases}$$

and

$$\int_{\mathbb{R}^n} x_i x_j x_k x_r\, e^{\frac{-|x|^2}{4}}\, dx = \begin{cases} 12\int\limits_{\mathbb{R}^n} e^{\frac{-|x|^2}{4}} dx, & i=j=k=r,\\ 4\int\limits_{\mathbb{R}^n} e^{\frac{-|x|^2}{4}} dx, & i=j\neq k=r,\\ 0, & else.\end{cases}$$

This implies

Corollary 23. *It holds that*

$$\frac{1}{2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} u_{ij}(0)\, z_i z_j \, d\tilde{z} \;=\; \Delta u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} d\tilde{z}.$$

Proof: We have

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} u_{ij}(0)\, z_i z_j \, d\tilde{z} &= \frac{1}{2}u_{ij}(0)\int_{\mathbb{R}^{n-1}} z_i z_j e^{\frac{-|\tilde{z}|^2}{4}} d\tilde{z} \\ &= \frac{1}{2}u_{ii}(0)\int_{\mathbb{R}^{n-1}} z_i^2 e^{\frac{-|\tilde{z}|^2}{4}} d\tilde{z} \\ &= \frac{1}{2}\Delta u(0)\cdot 2\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} d\tilde{z} \\ &= \Delta u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} d\tilde{z}\end{aligned}$$

since all the integrals containing mixed derivatives vanish by Corollary 22. □

We next prove the identity (2.11), i.e., that the coefficient a_2 is given by $\frac{1}{2}\Delta^2 u(0)$ and then show how to express $\frac{1}{2}\Delta^2 u(0)$ explicitly in terms of the geometric invariants $\triangle_{\partial D} H$, $H|A|^2$ and $\operatorname{tr} A^3$ (Proposition 25).

Proposition 24. *With a local normal representation of ∂D as graph of a smooth function u with $u(0) = p$ the coefficient a_2 is given by*

$$a_2 = \frac{1}{2}\Delta^2 u(0).$$

Proof: We have to prove that

$$\begin{aligned}&\frac{1}{24}\sum_{i,j,k,r} u_{ijkr}(0)\int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ =\;& \frac{1}{2}\Delta^2 u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}.\end{aligned}$$

By Corollary 22 we know that the integral $\int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}$ is non-zero if and only if it contains two (not necessarily different) pairs of coordinate directions. So

$$\begin{aligned}&\frac{1}{24}\sum_{i,j,k,r} u_{ijkr}(0)\int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ =\;& \frac{1}{24}\sum_{\substack{\text{two pairs}\\ \text{of indices}}} u_{ijkr}(0)\int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}. \qquad (2.12)\end{aligned}$$

Now clearly every summand containing four partial derivatives in the same coordinate direction appears only once in (2.12), and every derivative containing two pairs of *different* coordinate directions, i.e,

$$u_{iikk}(0), \qquad k > i,$$

appears $\binom{4}{2} = 6$ times for every combination of coordinate directions $i, k \in \{1, ..., n-1\}$. So the sum

$$\sum_{i}^{n-1} \sum_{k>i}^{n-1} u_{iikk}(0)$$

appears 6 times in (2.12) and therefore

$$\sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0)$$

exactly 3 times since we have now replaced $k > i$ by $k \neq i$. So we have

$$\sum_{\substack{\text{two pairs of} \\ \textit{different} \text{ indices}}} u_{ijkr}(0) = 3 \sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0)$$

and rewrite (2.12) as

$$\begin{aligned} & \frac{1}{24} \sum_{i,j,k,r} u_{ijkr}(0) \int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ = \; & \frac{1}{24} \Big[3 \sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0) \int_{\mathbb{R}^{n-1}} z_i^2 z_k^2 \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} + \sum_{i}^{n-1} u_{iiii}(0) \int_{\mathbb{R}^{n-1}} z_i^4 \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \Big]. \end{aligned}$$

Again by Corollary 22 we have that

$$\begin{aligned} \sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0) \int_{\mathbb{R}^{n-1}} z_i^2 z_k^2 \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} &= 4 \sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0) \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}, \\ \sum_{i}^{n-1} u_{iiii}(0) \int_{\mathbb{R}^{n-1}} z_i^4 \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} &= 12 \sum_{i}^{n-1} u_{iiii}(0) \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}. \end{aligned}$$

So we obtain

$$\begin{aligned} & \frac{1}{24} \sum_{i,j,k,r} u_{ijkr}(0) \int_{\mathbb{R}^{n-1}} z_i z_j z_k z_r \, e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ = \; & \frac{1}{24} \Big[3 \cdot 4 \sum_{i}^{n-1} \sum_{k\neq i}^{n-1} u_{iikk}(0) + 12 \sum_{i}^{n-1} u_{iiii}(0) \Big] \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ = \; & \frac{1}{24} \Big[12 \sum_{i}^{n-1} \sum_{k}^{n-1} u_{iikk}(0) \Big] \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z} \\ = \; & \frac{1}{2} \Delta^2 u(0) \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}} \, d\tilde{z}, \end{aligned}$$

which we wanted to prove. □

In order to complete the statement of Theorem 19 it remains to express $\frac{1}{2}\Delta^2 u(0)$ in terms of the geometric invariants $\triangle_{\partial D} H$, $H|A|^2$ and $\operatorname{tr} A^3$.

Proposition 25. *Let ∂D at $p \in \partial D$ in normal coordinates be locally represented as graph of a smooth function u with $u(0) = p$. Then we have the following identity*

$$a_2 = \frac{1}{2}\Delta^2 u(0) = -\frac{1}{2}(\triangle_{\partial D} H + H|A|^2 + 2\,\mathrm{tr}\,A^3)\Big|_p,$$

where $\triangle_{\partial D}$ is the Laplace-Beltrami operator, H the mean curvature and A the second fundamental form of the boundary ∂D.

Proof: In the following we denote by $\partial_k h_{ij}$ the coordinate derivative of the second fundamental form, by $\nabla_k h_{ij}$ its covariant derivative and by $D_k u$ the coordinate derivatives of the function u. We again use the sum convention.

We start with the second fundamental form h_{ij} of ∂D at p and determine first its second covariant derivative $\nabla_r \nabla_k h_{ij}$.

By definition of the Christoffel symbols, the first covariant derivative of h_{ij} is

$$\nabla_k h_{ij} = \partial_k h_{ij} - \Gamma^l_{ki} h_{lj} - \Gamma^l_{kj} h_{li}.$$

So the second covariant derivative of h_{ij} at p is given by

$$\begin{aligned}
\nabla_r \nabla_k h_{ij}\Big|_p &= \partial_r(\partial_k h_{ij} - \Gamma^l_{ki} h_{lj} - \Gamma^l_{kj} h_{li}) - 0 \\
&= \partial_r \partial_k h_{ij} - \partial_r \Gamma^l_{ki} h_{lj} - \partial_r \Gamma^l_{kj} h_{li} - \underbrace{\Gamma^l_{ki}\partial_r h_{lj} - \Gamma^l_{kj}\partial_r h_{li}}_{=0} \qquad (2.13)\\
&= \partial_r \partial_k h_{ij} - \partial_r \Gamma^l_{ki} h_{lj} - \partial_r \Gamma^l_{kj} h_{li},
\end{aligned}$$

since the Christoffel symbols Γ^k_{ij} vanish at p.

Since $h_{ij} = \frac{-D_i D_j u}{\sqrt{1+|Du|^2}}$, we compute the second coordinate derivative of h_{ij} as

$$\begin{aligned}
\partial_r \partial_k h_{ij} &= D_r D_k \Big(\frac{-D_i D_j u}{\sqrt{1+|Du|^2}}\Big) \\
&= D_r \Big(\frac{-D_k D_i D_j u}{\sqrt{1+|Du|^2}} + \frac{1}{2}\frac{D_i D_j u \cdot 2 \cdot D_l u \cdot D_l D_k u}{(1+|Du|^2)^{3/2}}\Big) \\
&= -\frac{D_r D_k D_i D_j u}{\sqrt{1+|Du|^2}} + \frac{1}{2}\frac{\overbrace{D_k D_i D_j u \cdot 2 \cdot D_l u \cdot D_l D_r u}^{=0}}{(1+|Du|^2)^{3/2}} \\
&\quad + \frac{\overbrace{D_r D_i D_j u \cdot D_l u \cdot D_l D_k u}^{=0} + D_i D_j u \cdot D_r D_l u \cdot D_l D_k u + \overbrace{D_i D_j u \cdot D_l u \cdot D_r D_l D_k u}^{=0}}{(1+|Du|^2)^{3/2}} \\
&\quad - \overbrace{\frac{3}{2}\frac{D_i D_j u \cdot D_l u \cdot D_l D_k u \cdot 2 \cdot D_k u \cdot D_k D_r u}{(1+|Du|^2)^{5/2}}}^{=0},
\end{aligned}$$

where for the parentheses we have used that $Du = 0$ at p, so $\sqrt{1+|Du|^2} = 1$ and every factor that contains a first derivative of u vanishes. So we obtain

$$\partial_r \partial_k h_{ij}\Big|_p = -D_r D_k D_i D_j u + D_i D_j u \cdot D_r D_l u \cdot D_l D_k u. \qquad (2.14)$$

Now we compute the terms $\partial_r \Gamma^l_{ki} h_{lj}$ and $\partial_r \Gamma^l_{kj} h_{li}$ of (2.13). Recall that the first derivative of g_{ij} at p is given by

$$\partial_k g_{ij} \;=\; D_k D_i u \cdot D_j u + D_i u \cdot D_k D_j u \;=\; 0. \tag{2.15}$$

Since we want to compute the first derivative of the Christoffel symbols Γ^k_{ij}, we determine the second derivative of g_{ij} in terms of the representation u:

$$\begin{aligned} \partial_r \partial_k g_{ij}\Big|_p &= D_r(D_k D_i u \cdot D_j u + D_i u \cdot D_k D_j u) \\ &= \underbrace{D_r D_k D_i u \cdot D_j u}_{=0} + D_k D_i u \cdot D_r D_j u + D_r D_i u \cdot D_k D_j u + \underbrace{D_i u \cdot D_r D_k D_j u}_{=0} \\ &= D_k D_i u \cdot D_r D_j u + D_r D_i u \cdot D_k D_j u. \end{aligned} \tag{2.16}$$

Using (2.15) and (2.16) we obtain the first derivative of the Christoffel symbols as

$$\begin{aligned} \partial_r \Gamma^k_{ij}\Big|_p &= \partial_r \Big(\frac{1}{2} g^{kl} \Big(\partial_i g_{jl} + \partial_j g_{il} - \partial_l g_{ij} \Big) \Big) \\ &= \frac{1}{2} \delta^{kl} \Big(\partial_r \partial_i g_{jl} + \partial_r \partial_j g_{il} - \partial_r \partial_l g_{ij} \Big) \\ &= \frac{1}{2} \Big(\partial_r \partial_i g_{jk} + \partial_r \partial_j g_{ki} - \partial_r \partial_k g_{ij} \Big) \\ &= \frac{1}{2} \Big(D_i D_j u \cdot D_r D_k u + D_r D_j u \cdot D_i D_k u \\ &\qquad + D_j D_k u \cdot D_r D_i u + D_r D_k u \cdot D_j D_i u \\ &\qquad - D_k D_i u \cdot D_r D_j u - D_r D_i u \cdot D_k D_j u \Big) \\ &= \frac{1}{2} \Big(D_i D_j u \cdot D_r D_k u + D_r D_k u \cdot D_j D_i u \Big) \\ &= D_i D_j u \cdot D_r D_k u, \end{aligned}$$

and therefore with $h_{ij} = -D_i D_j u$ at p

$$-\partial_r \Gamma^l_{ki} h_{lj}\Big|_p - \partial_r \Gamma^l_{kj} h_{li}\Big|_p \;=\; D_k D_i u \cdot D_r D_l u \cdot D_l D_j u + D_k D_j u \cdot D_r D_l u \cdot D_l D_i u. \tag{2.17}$$

We now put (2.14) and (2.17) in (2.13) and obtain the second covariant derivative of the second fundamental form in the point p in terms of u as

$$\begin{aligned} \nabla_r \nabla_k h_{ij}\Big|_p &= \partial_r \partial_k h_{ij} - \partial_r \Gamma^l_{ki} h_{lj} - \partial_r \Gamma^l_{kj} h_{li} \\ &= -D_r D_k D_i D_j u + D_i D_j u \cdot D_r D_l u \cdot D_l D_k u \\ &\quad + D_k D_i u \cdot D_r D_l u \cdot D_l D_j u + D_k D_j u \cdot D_r D_l u \cdot D_l D_i u. \end{aligned}$$

So we obtain

$$D_r D_k D_i D_j u \;=\; -\nabla_r \nabla_k h_{ij} - h_{ij} h_{rl} h_{lk} - h_{ki} h_{rl} h_{lj} - h_{kj} h_{rl} h_{li}.$$

Finally, taking the sum over $k = r$ and $i = j$, we have

$$\begin{aligned} D_k D_k D_i D_i u &= -\Big(\nabla_k \nabla_k h_{ii} + h_{ii} h_{kl} h_{lk} + h_{ki} h_{kl} h_{li} + h_{ki} h_{kl} h_{li} \Big) \\ &= -\Big(\nabla_k \nabla_k h_{ii} + h_{ii} h_{kl} h_{lk} + 2 h_{ik} h_{kl} h_{li} \Big), \end{aligned}$$

which by $H|A|^2 = h_{ii}h_{kl}h_{lk}$ and $\operatorname{tr} A^3 = h_{ik}h_{kl}h_{li}$ yields

$$\Delta^2 u(0) = -(\triangle_{\partial D} H + H|A|^2 + 2\operatorname{tr} A^3)\Big|_p,$$

what we wanted to prove. □

This now completes the proof of all statements of Theorem 19.

2.1.2 Higher order coefficients

Observe that by taking more summands in the Taylor series expansion (2.9) in the proof of Theorem 19 we can determine also higher order coefficients a_k of the asymptotics. By the symmetry of Gaussian integrals it follows immediately that $a_k = 0$ if k is fractional. Whereas a_k (k integer) is implicitly given by

$$\frac{1}{(2k)!}\sum_{r_1,\dots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \;=\; a_k\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z}.$$

We determine a general formula how to compute a_k from the function u. Therefore, we first provide a representation formula for the k-th power of the Laplacian that will be essential in the proof of Theorem 27.

Lemma 26. *Let Δ be the standard Laplacian on $C^\infty(\mathbb{R}^{n-1})$. Then the k-th power Δ^k of the Laplacian applied to a function $u \in C^\infty(\mathbb{R}^{n-1})$, i.e.,*

$$\Delta^k u = \sum_{r_1,r_2,\dots,r_k=1}^{n-1} D^2_{r_1}D^2_{r_2}\cdots D^2_{r_k}u, \tag{2.18}$$

can be represented as

$$\Delta^k u \;=\; \sum_{(q_1,\dots,q_m)\in Q_m}\frac{k!}{\prod_{i=1}^{m} q_i!}\sum_{r_1\neq r_2\neq\dots\neq r_m=1}^{n-1}\underbrace{(D^2_{r_1})^{q_1}(D^2_{r_2})^{q_2}\cdots(D^2_{r_m})^{q_m}u}_{2k\ \text{derivatives}} \tag{2.19}$$

$$=\; \sum_{q\in Q_m} A_k(q)\sum_{r\in R_m} D^{2q}u, \tag{2.20}$$

where

$$m := \min\{k, n-1\}.$$

Here, Q_m is the set of all ordered multi-indices $(q_1,\dots,q_m)\in\mathbb{N}^m$ of length k, i.e.,

$$Q_m := \{q = (q_1,\dots,q_m)\in\mathbb{N}^m : 0\le q_1\le q_2\le\dots\le q_m \text{ and } q_1+\dots+q_m = k\}$$

and R_m is the set of all m-tuples of coordinate directions in $\mathbb{R}^{n-1}$ with pairwise different entries, i.e.,

$$R_m := \{(r_1,r_2,\dots,r_m)\in\{1,2,\dots,n-1\}^m : r_1\neq r_2\neq\dots\neq r_m\}$$

(since $m\le n-1$, R_m is well defined).

Proof: By (2.18), the k-th power of the Laplacian is given by the sum of partial derivatives, where each summand contains k pairs of squares of partial derivatives. Since in each summand of (2.18) every partial derivative appears an even number of times, every summand can have at most k pairwise different partial derivatives. On the other side, since u depends on $n-1$ variables, each summand can contain at most $n-1$ pairwise different partial derivatives. So the maximal number of pairwise different partial derivatives in each summand is

$$m = \min\{k, n-1\}.$$

Since $u \in C^\infty(\mathbb{R}^{n-1})$ all partial derivatives commute. The expression (2.19) is therefore a representation of $\Delta^k u$ where all the partial derivatives are already "sorted" in the sense that in every summand all appearing partial derivatives in the same coordinate direction are iterated correspondingly to their multiplicity and ordered by their multiplicity $0 \leq q_1 \leq q_2 \leq ... \leq q_m$.
It then only remains to determine the multiplicity of each of these "sorted" partial derivatives

$$D^{2q}u = D_{r_1}^{2q_1} D_{r_2}^{2q_2} \cdots D_{r_m}^{2q_m} u, \tag{2.21}$$

i.e., to determine how often we have a summand in (2.18) that contains q_1 squares of derivatives in coordinate direction r_1, q_2 squares of derivatives in coordinate direction r_2, and so on.
This multiplicity can now be calculated by the combinatorical expression

$$\begin{aligned} A_k(q) &:= \binom{k}{q_1}\binom{k-q_1}{q_2}\cdots\binom{k-\sum_{i=1}^{m-1} q_i}{q_m} \\ &= \frac{k\ldots(k-q_1+1)}{q_1!}\cdot\frac{(k-q_1)\ldots(k-q_1-q_2+1)}{q_2!}\cdot\ldots\cdot\frac{\left(k-\sum_{i=1}^{m-1} q_i\right)!}{q_m!} \\ &= \frac{k!}{\prod_{i=1}^{m} q_i!}. \end{aligned}$$

The assertion now follows by taking the sum over all possible combinations of different partial derivatives, i.e., $q \in Q_m$, and all pairwise different coordinate directions, i.e., $r \in R_m$, with the corresponding multiplicity $A_k(q)$, i.e.,

$$\Delta^k u = \sum_{(q_1,\ldots,q_m)\in Q_m} \frac{k!}{\prod_{i=1}^{m} q_i!} \sum_{r_1\neq r_2\neq\ldots\neq r_m=1}^{n-1} \underbrace{(D_{r_1}^2)^{q_1}(D_{r_2}^2)^{q_2}\cdots(D_{r_m}^2)^{q_m}u}_{2k\,derivatives}. \qquad \square$$

We can now state and prove the generalisation of Proposition 24 to higher order coefficients a_k.

Proposition 27. *Let ∂D at $p \in \partial D$ in normal coordinates be locally represented as graph of a smooth function u with $u(0) = p$. Then the coefficient a_k (k integer) in the expansion of the normal distance function $d_\lambda(t)$ describing the evolution of the level sets $D_\lambda(t)$ is given by*

$$a_k = \frac{1}{k!}\,\Delta^k u(0).$$

Proof: Starting from the Taylor expansion (2.9) we have to show that

$$\underbrace{\frac{1}{(2k)!}\sum_{r_1,\ldots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\overbrace{\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z}^{(B)}}_{(A)} \tag{2.22}$$
$$= \frac{1}{k!}\,\Delta^k u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z.$$

For this purpose, we look at the combinatorical structure of the sum (A), and at symmetry properties of the integral (B).

Since by Proposition 21 the integral (B) is zero if and only if one of the $2k$ coordinate directions $r_1, ..., r_{2k} \in \{1, ..., n-1\}$ occurs an *odd* number of times, the sum (A) in fact only contains summands where each of the coordinate directions $r_1, ..., r_{2k}$ appears an even number of times. So we have

$$\sum_{r_1,\ldots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z$$
$$= \sum_{\substack{k \text{ pairs of}\\ \text{indices}}} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z.$$

Now, by the same arguments as in the proof of Lemma 26, every summand in (2.22) contains at most $m = \min\{k, n-1\}$ pairwise different partial derivatives and hence can be written as

$$D_{r_1}^{2q_1}D_{r_2}^{2q_2}\cdots D_{r_m}^{2q_m}u, \tag{2.23}$$

where $r_1 \neq r_2 \neq ... \neq r_m \in \{1, 2, ..., n-1\}$ are pairwise different coordinate directions and $q_1 \leq q_2 \leq ... \leq q_m$ are the corresponding multiplicities of partial derivatives in these directions.

Next we determine how often each of these derivatives actually appears in the sum (2.22) after we have "sorted" the partial derivatives. We denote by $M(q)$ the multiplicity of summands in (2.22) that are of the form (2.23) for a given $q = (q_1, ..., q_m)$. This yields

$$\sum_{r_1,\ldots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z$$
$$= \sum_{q\in Q_m} M(q)\sum_{r_1\neq r_2\neq\ldots\neq r_m=1}^{n-1} \underbrace{D_{r_1}^{2q_1}D_{r_2}^{2q_2}\cdots D_{r_m}^{2q_m}u(0)}_{2k\, derivatives}\int_{\mathbb{R}^{n-1}} z_{r_1}^{2q_1}z_{r_2}^{2q_2}\cdots z_{r_m}^{2q_m}\, e^{\frac{-|\tilde z|^2}{4}}\, d\tilde z.$$

Now, determining the value of $M(q) = M(q_1, ..., q_m)$ reduces to the combinatorical question how many possibilities do we have to distribute $2q_1$ times an index r_1, $2q_2$

times an index r_2, ..., and $2q_m$ times an index r_m on alltogether $2k$ positions. Therefore

$$\begin{aligned}
M(q) &= \underbrace{\binom{2k}{2q_1}\binom{2k-2q_1}{2q_2}\binom{2k-2q_1-2q_2}{2q_3}\cdot\ldots\cdot\binom{2k-\sum\limits_{i=1}^{m-1}2q_i}{2q_m}}_{m\text{ factors}} \\
&= \frac{(2k)\cdot\ldots\cdot(2k-2q_1+1)}{(2q_1)!}\cdot\ldots\cdot\frac{(2k-\sum\limits_{i=1}^{m-1}2q_i)\cdot\ldots\cdot 1}{(2q_m)!} \\
&= \frac{(2k)!}{\prod\limits_{i=1}^{m}(2q_i)!}.
\end{aligned}$$

Further, we have by Proposition 21 that

$$\int_{\mathbb{R}^{n-1}} z_{r_1}^{2q_1} z_{r_2}^{2q_2}\cdots z_{r_m}^{2q_m}\, e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \;=\; I(q)\cdot\int\limits_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z}$$

with

$$I(q) = \prod_{i=1}^{m}\frac{(2q_i)!}{(q_i)!}.$$

So we obtain

$$\begin{aligned}
&\sum_{r_1,\ldots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \\
&= \sum_{q\in Q_m} M(q) \sum_{r_1\neq r_2\neq\ldots\neq r_m=1}^{n-1} D_{r_1}^{2q_1}D_{r_2}^{2q_2}\cdots D_{r_m}^{2q_m}u(0)\cdot I(q)\int\limits_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \\
&= \sum_{q\in Q_m} M(q)\cdot I(q)\sum_{r\in R_m} D^{2q}u(0)\int\limits_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z},
\end{aligned}$$

with

$$\begin{aligned}
Q_m &= \{q\in\mathbb{N}^m : 0\le q_1\le q_2\le\ldots\le q_m \text{ and } q_1+\ldots+q_m=k\} \\
R_m &= \{(r_1,r_2,\ldots,r_m)\in\{1,2,\ldots,n-1\}^m : r_1\neq r_2\neq\ldots\neq r_m\}
\end{aligned}$$

as in Lemma 26.

Now the product $M(q)\cdot I(q)$ is given as

$$M(q)\cdot I(q) = \frac{(2k)!}{\prod\limits_{i=1}^{m}(2q_i)!}\cdot\prod_{i=1}^{m}\frac{(2q_i)!}{(q_i)!} = \frac{(2k)!}{\prod\limits_{i=1}^{m}q_i!},$$

and we therefore finally obtain

$$\begin{aligned}
&\sum_{r_1,\ldots,r_{2k}=1}^{n-1} D_{r_1}D_{r_2}\cdots D_{r_{2k}}u(0)\int_{\mathbb{R}^{n-1}} z_{r_1}z_{r_2}\cdots z_{r_{2k}}\, e^{\frac{-|\tilde z|^2}{4}}\,d\tilde z\\
&= \sum_{q\in Q_m} M(q)\cdot I(q)\sum_{r\in R_m} D^{2q}u(0)\int\limits_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}}\,d\tilde z\\
&= \sum_{(q_1,\ldots,q_m)\in Q_m}\frac{(2k)!}{\prod_{i=1}^m q_i!}\sum_{r_1\neq r_2\neq\ldots\neq r_m=1}^{n-1} D_{r_1}^{2q_1}D_{r_2}^{2q_2}\cdots D_{r_m}^{2q_m}u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}}\,d\tilde z\\
&= \frac{(2k)!}{k!}\underbrace{\sum_{(q_1,\ldots,q_m)\in Q_m}\frac{k!}{\prod_{i=1}^m q_i!}\sum_{r_1\neq r_2\neq\ldots\neq r_m=1}^{n-1} D_{r_1}^{2q_1}D_{r_2}^{2q_2}\cdots D_{r_m}^{2q_m}u(0)}_{=\Delta^k u(0)}\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}}\,d\tilde z\\
&= \frac{(2k)!}{k!}\Delta^k u(0)\int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde z|^2}{4}}\,d\tilde z
\end{aligned}$$

by the representation of $\Delta^k u$ from Lemma 26. Dividing by $(2k)!$ then yields the assertion. □

2.2 Heat diffusion into the complement

2.2.1 Compact sets with smooth boundary

We now derive from the results above the short time behaviour of the map

$$t \mapsto \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle,$$

i.e., the short time behaviour for the amount of heat that has flowed from D into the complement D^c after time t.

We prove that for a compact set D with smooth boundary the equality

$$\lim_{t\to 0}\frac{\sqrt{\pi}}{\sqrt{t}}\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = P(D)$$

holds, which generalises the result M. Ledoux obtained for Euclidean balls (see Chapter 1, Proposition 13).

The basic idea is to look at the superlevel sets of $T(t)\mathbb{1}_D$ defined as follows.

Definition 28. For $\lambda \in (0,1)$ we call

$$D^\lambda(t) := \{x\in\mathbb{R}^n : T(t)\mathbb{1}_D(x)\geq\lambda\},\qquad t>0,$$

the *superlevel set of* $T(t)\mathbb{1}_D$ *for the level* λ.

We proceed in two steps: Up to an $O(t)$ we approximate the volume of $D^\lambda(t)$ as $t \to 0$ and then integrate over all levels that yield a contribution to the heat in the complement.

Therefore, we first look at the behaviour of the volume of so called parallel sets.

Definition 29. Let $D \subset \mathbb{R}^n$ be a compact set with smooth boundary. We call

$$D_r := \{x \in \mathbb{R}^n : \operatorname{dist}(D, x) \leq r\}, \qquad r > 0,$$

the *parallel sets* of D.

Remark 30. For r smaller than the injectivity radius of ∂D the boundaries of D_r are smooth and given by

$$\partial D_r = \{x + r \cdot \nu(x) : x \in \partial D\}.$$

The following expansion of the volume $|D_r|$ should be known, but we have not found an explicit reference in the literature.

Proposition 31. *The volume of D_r has the following expansion*

$$|D_r| \;=\; |D| + r \cdot P(D) + \frac{r^2}{2} \int_{\partial D} H \, d\sigma + O(r^3) \qquad \text{as } r \to 0. \tag{2.24}$$

Proof: In order to obtain the expansion we deduce the first and second derivative of $r \mapsto |D_r|$ at $r = 0$ from the first and second variation of volume formulas (see e.g. [Spi79, Volume 4, Chapter 9], [Met02]).

For a smooth variation $F : \mathbb{R}^n \times (-\varepsilon, \varepsilon) \to \mathbb{R}^n$ of D with variational vector field $X_r = \frac{dF}{dr}$ the first variation of the volume of $F(D, r)$ is given by

$$\frac{d}{dr}\Big|_{r=0} |F(D, r)| = \int_{\partial D} \langle X_0, \nu \rangle \, d\sigma,$$

i.e., we integrate the normal velocity $\langle X_0, \nu \rangle$, ν the outer unit normal, at $r = 0$ over ∂D. In our situation we simply have $X_0 = \nu$ (i.e., normal velocity constant to 1), so

$$\frac{d}{dr}\Big|_{r=0} |D_r| = \int_{\partial D} \langle \nu, \nu \rangle \, d\sigma = P(D). \tag{2.25}$$

The second variation of $|F(D, r)|$ is given by

$$\frac{d^2}{dr^2}\Big|_{r=0} |F(D, r)| \;=\; \int_{\partial D} \frac{d}{dr} \langle X_r, \nu \rangle \Big|_{r=0} + \langle X_0, \nu \rangle \operatorname{div} X_0 \, d\sigma.$$

In our case we have $X_r = \nu$, hence $\langle X_r, \nu \rangle = 1$ and $\frac{d}{dr} \langle X_r, \nu \rangle \Big|_{r=0} = 0$. So it holds

$$
\begin{aligned}
\frac{d^2}{dr^2}\Big|_{r=0} |D_r| &= \int_{\partial D} \operatorname{div} \nu \, d\sigma \\
&= \int_{\partial D} H \, d\sigma,
\end{aligned} \tag{2.26}
$$

since the divergence of the normal vector field on ∂D is its mean curvature H.
By (2.25) and (2.26) we obtain from Taylor's theorem that

$$
|D_r| = |D| + r \cdot P(D) + \frac{r^2}{2} \int_{\partial D} H \, d\sigma + O(r^3) \qquad \text{as } r \to 0. \quad \Box
$$

We can now prove the following result.

Theorem 32. *Let $D \subset \mathbb{R}^n$ be a compact set with smooth boundary. Then*

$$
\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c} \rangle = \frac{\sqrt{t}}{\sqrt{\pi}} \cdot P(D) + O(t) \qquad \textit{as } t \to 0.
$$

In particular we have

$$
\lim_{t \to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c} \rangle = P(D).
$$

Proof: From the asymptotic behaviour of the normal distance function

$$
d_\lambda(t) = -t^{1/2} c_\lambda + O(t)
$$

and its square

$$
d_\lambda^2(t) = t c_\lambda^2 + O(t^{3/2})
$$

it is clear that only $d_\lambda(t)$ (and not its square) yields a contribution of order $t^{1/2}$ for the volume of $D^\lambda(t)$. Therefore, as $t \to 0$ the volume $|D^\lambda(t)|$ behaves up to an $O(t)$ as the volume of the parallel set D_r with $r = -t^{1/2} c_\lambda$.
So with Proposition 31 we obtain

$$
\begin{aligned}
|D^\lambda(t)| &= D_{-t^{1/2} c_\lambda} + O(t) \\
&= |D| - t^{1/2} c_\lambda P(D) + O(t) \qquad \text{as } t \to 0.
\end{aligned}
$$

Since for small t the level set $D_\lambda(t)$ is the boundary of the superlevel set $D^\lambda(t)$, the asymptotic expansion of the normal distance $d_\lambda(t)$ yields for small t that

$$
\begin{aligned}
D^\lambda(t) &\subset D, & \lambda \in (\tfrac{1}{2}, 1), \\
D &\subset D^\lambda(t), & \lambda \in (0, \tfrac{1}{2}).
\end{aligned}
$$

So we obtain the asymptotic behaviour of $t \mapsto \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle$ as $t \to 0$ by integrating the volume of all superlevel sets $\lambda \in (0, \frac{1}{2})$ and then subtracting $\frac{1}{2}|D|$, i.e.,

$$\begin{aligned}\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle &= \int_0^{1/2} |D| - t^{1/2} \cdot P(D) c_\lambda \, d\lambda - \frac{1}{2}|D| + O(t) \\ &= -t^{1/2} \cdot P(D) \int_0^{1/2} c_\lambda \, d\lambda + O(t).\end{aligned}$$

It remains to determine the integral

$$-\int_0^{1/2} c_\lambda \, d\lambda.$$

Therefore, observe that $c_\lambda = \Phi^{-1}(\lambda)$, i.e., c_λ considered as a function of λ is the inverse of Φ (cf. Definition 15), and $\Phi(-x) = 1 - \Phi(x)$. So we have

$$-\int_0^{1/2} c_\lambda \, d\lambda = \int_{-\infty}^{0} \Phi(x) \, dx = \int_0^{\infty} (1 - \Phi(x)) \, dx.$$

From [GR65, 6.281] we take the identity

$$\int_0^{\infty} (1 - \Phi(p\, x)) x^{2q-1} \, dx = \frac{\Gamma(q + \frac{1}{2})}{2\sqrt{\pi}\, q\, p^{2q}},$$

which implies

$$-\int_0^{1/2} c_\lambda \, d\lambda = \int_0^{\infty} (1 - \Phi(x)) \, dx = \frac{1}{\sqrt{\pi}} \qquad \text{for } q = \frac{1}{2}, p = 1.$$

This finally yields

$$\begin{aligned}\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle &= -t^{1/2} \cdot P(D) \int_0^{1/2} c_\lambda \, d\lambda + O(t) \\ &= \frac{\sqrt{t}}{\sqrt{\pi}} \cdot P(D) + O(t). \qquad \text{as } t \to 0.\end{aligned}$$

□

2.2.2 Caccioppoli sets

We now drop the smoothness assumptions on the boundary and study the heat flow $t \mapsto \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle$ for a Caccioppoli set D. We show that for every Caccioppoli set $D \subset \mathbb{R}^n$ it holds

$$\lim_{t \to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = P(D).$$

Although this result yields the desired assertion for much more sets than Theorem 32, we obtain less insight into the "geometric nature" of the flow.

Let us first study the short time behaviour of the semigroup $(T(t))_{t\geq 0}$ with respect to two arbitrary Caccioppoli sets.

Proposition 33. *For two Caccioppoli sets $A, D \subset \mathbb{R}^n$ the equality*

$$\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_A \rangle = \int\limits_{\mathcal{F}A\cap\mathcal{F}D} \langle \nu_A(x), \nu_D(x) \rangle \, d\mathcal{H}^{n-1}(x) \tag{2.27}$$

holds.

Proof: Since

$$T(t)\mathbb{1}_D - \mathbb{1}_D = \int\limits_0^t \Delta T(s)\mathbb{1}_D \, ds,$$

we have

$$\langle T(t)\mathbb{1}_D - \mathbb{1}_D, \mathbb{1}_A \rangle = \langle \int\limits_0^t \Delta T(s)\mathbb{1}_D \, ds, \mathbb{1}_A \rangle = \int\limits_0^t \langle \Delta T(s)\mathbb{1}_D, \mathbb{1}_A \rangle \, ds.$$

Moreover, by the generalised Gauß-Green formula for Caccioppoli sets (see Chapter 1, Section 1.1) we obtain

$$\begin{aligned} \langle \Delta T(s)\mathbb{1}_D, \mathbb{1}_A \rangle &= \int\limits_A \Delta T(s)\mathbb{1}_D(x) \, dx \\ &= -\int\limits_{\mathcal{F}A} \langle \nabla T(s)\mathbb{1}_D(x), \nu_A(x) \rangle \, d\mathcal{H}^{n-1}(x) \end{aligned}$$

for the reduced boundary $\mathcal{F}A$ of A. So

$$\langle T(t)\mathbb{1}_D - \mathbb{1}_D, \mathbb{1}_A \rangle = -\int\limits_0^t \int\limits_{\mathcal{F}A} \langle \nabla T(s)\mathbb{1}_D(x), \nu_A(x) \rangle \, d\mathcal{H}^{n-1}(x) \, ds$$

and clearly

$$\langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_A \rangle = \int\limits_0^t \int\limits_{\mathcal{F}A} \langle \nabla T(s)\mathbb{1}_D(x), \nu_A(x) \rangle \, d\mathcal{H}^{n-1}(x) \, ds.$$

Notice that, if we define for $x \in \mathbb{R}^n$ and $s > 0$ the measures

$$d\mu_{s,x} := \mathcal{L}^n \llcorner \left(\frac{D - x}{\sqrt{s}} \right),$$

we have

$$\begin{aligned}\nabla T(s)\mathbb{1}_D(x) &= \int\limits_D \nabla\Big(\frac{1}{(4\pi s)^{n/2}}\, e^{\frac{-|x-y|^2}{4s}}\Big)\, dy = -\int\limits_D \frac{(x-y)}{2s\,(4\pi s)^{n/2}}\, e^{\frac{-|x-y|^2}{4s}}\, dy \\ &= \frac{1}{2\sqrt{s}} \int\limits_{\frac{D-x}{\sqrt{s}}} z\, \frac{1}{(4\pi)^{n/2}}\, e^{\frac{-|z|^2}{4}}\, dz \\ &= \frac{1}{2\sqrt{s}} \int\limits_{\mathbb{R}^n} z\, \frac{1}{(4\pi)^{n/2}}\, e^{\frac{-|z|^2}{4}}\, d\mu_{s,x}(z).\end{aligned}$$

Moreover, for every $x \in \mathcal{F}D$ we define the half space

$$H_{\nu_D(x)} := \{z \in \mathbb{R}^n : \langle z, \nu_D(x)\rangle \geq 0\}\,.$$

By the existence of the approximate tangent space for $x \in \mathcal{F}D$ (see Chapter 1, Section 1.3) the measures $\mu_{s,x}$, for $x \in \mathcal{F}D$, are locally weak* convergent as $s \to 0$ to the Lebesgue measure $\mathcal{L}^n$ restricted to $H_{\nu_D(x)}$

$$d\mu_x := \mathcal{L}^n \llcorner H_{\nu_D(x)},$$

in the sense that

$$\lim_{s\to 0} \int\limits_{\mathbb{R}^n} \varphi\, d\mu_{s,x} = \int\limits_{\mathbb{R}^n} \varphi\, d\mu_x, \qquad\qquad \varphi \in C_c(\mathbb{R}^n).$$

We observe that, although the function $z \mapsto \langle z, \nu_A(x)\rangle\, e^{\frac{-|z|^2}{4}}$ does not have compact support, but decreases fast enough, it holds

$$\lim_{s\to 0} \int\limits_{\mathbb{R}^n} \langle z, \nu_A(x)\rangle e^{\frac{-|z|^2}{4}}\, d\mu_{s,x}(z) = \begin{cases} \int\limits_{H_{\nu_D(x)}} \langle z, \nu_A(x)\rangle\, e^{\frac{-|z|^2}{4}}\, dz, & x \in \mathcal{F}D, \\ \int\limits_{\mathbb{R}^n} \langle z, \nu_A(x)\rangle\, e^{\frac{-|z|^2}{4}}\, dz, & x \in D^1, \\ 0, & x \in D^0. \end{cases}$$

Further, the second integral is always zero: By rotational invariance we may assume that $\nu_A = e_n$, so

$$\int\limits_{\mathbb{R}^n} \langle z, \nu_D(x)\rangle\, e^{\frac{-|z|^2}{4}}\, dz \;=\; \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \underbrace{\int_{-\infty}^{\infty} z_n\, e^{\frac{-z_n^2}{4}}\, dz_n}_{=0} = 0.$$

Therefore

$$\lim_{s\to 0} \int\limits_{\mathbb{R}^n} \langle z, \nu_A(x)\rangle e^{\frac{-|z|^2}{4}}\, d\mu_{s,x}(z) = \begin{cases} \int\limits_{H_{\nu_D(x)}} \langle z, \nu_A(x)\rangle\, e^{\frac{-|z|^2}{4}}\, dz, & x \in \mathcal{F}D, \\ 0, & x \in (D^0 \cup D^1). \end{cases} \tag{2.28}$$

Altogether we write

$$\frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_A \rangle = \int_{\mathcal{F}A} g(x,t)\, d\mathcal{H}^{n-1}(x),$$

where $g : \mathcal{F}A \times (0,\infty) \to \mathbb{R}$ is given by

$$g(x,t) := \frac{\sqrt{\pi}}{\sqrt{t}} \int_0^t \frac{1}{2\sqrt{s}} \int_{\mathbb{R}^n} \langle z, \nu_A(x) \rangle \frac{1}{(4\pi)^{n/2}}\, e^{\frac{-|z|^2}{4}}\, d\mu_{s,x}(z)\, ds.$$

By (2.28) and $\mathcal{H}^{n-1}(\mathbb{R}^n \setminus [D^0 \cup D^1 \cup \mathcal{F}D]) = 0$, see (1.8), we obtain the limit

$$\lim_{t\to 0} g(x,t) = \begin{cases} \dfrac{\sqrt{\pi}}{(4\pi)^{n/2}} \displaystyle\int_{H_{\nu_D(x)}} \langle z, \nu_A(x) \rangle\, e^{\frac{-|z|^2}{4}} dz & \text{for } x \in \mathcal{F}A \cap \mathcal{F}D, \\ 0 & \text{for } x \in \mathcal{F}A \cap (D^0 \cup D^1). \end{cases}$$

Note that $|g(x,t)|$ is bounded from above by

$$|g(x,t)| \le \frac{\sqrt{\pi}}{(4\pi)^{n/2}} \int_{\mathbb{R}^n} |z|\, e^{\frac{-|z|^2}{4}}\, dz = \text{const.}$$

So we can apply Lebesgue's dominated convergence theorem and obtain

$$\begin{aligned} &\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_A \rangle \\ = \;& \frac{\sqrt{\pi}}{(4\pi)^{n/2}} \int_{\mathcal{F}A\cap\mathcal{F}D} \int_{H_{\nu_D(x)}} \langle z, \nu_A(x) \rangle\, e^{\frac{-|z|^2}{4}}\, dz\, d\mathcal{H}^{n-1}(x) \\ = \;& \frac{\sqrt{\pi}}{(4\pi)^{n/2}} \int_{\mathcal{F}A\cap\mathcal{F}D} \int_{H_{\nu_D(x)}} \langle \nu_A(x), \nu_D(x) \rangle \langle z, \nu_D(x) \rangle\, e^{\frac{-|z|^2}{4}}\, dz\, d\mathcal{H}^{n-1}(x) \\ = \;& \int_{\mathcal{F}A\cap\mathcal{F}D} \langle \nu_A(x), \nu_D(x) \rangle \frac{\sqrt{\pi}}{(4\pi)^{n/2}} \int_{H_{\nu_D(x)}} \langle z, \nu_D(x) \rangle\, e^{\frac{-|z|^2}{4}}\, dz\, d\mathcal{H}^{n-1}(x) \\ = \;& \int_{\mathcal{F}A\cap\mathcal{F}D} \langle \nu_A(x), \nu_D(x) \rangle\, d\mathcal{H}^{n-1}(x), \end{aligned}$$

since $\langle \nu_A(x), \nu_D(x) \rangle\, \nu_D(x) = \nu_A(x)$ for $\mathcal{H}^{n-1}$-a.e. $x \in \mathcal{F}A \cap \mathcal{F}D$ (because $\nu_A(x)$ and $\nu_D(x)$ are parallel for $\mathcal{H}^{n-1}$-a.e. $x \in \mathcal{F}A \cap \mathcal{F}D$) and

$$\frac{\sqrt{\pi}}{(4\pi)^{n/2}} \int_{H_{\nu_D(x)}} \langle z, \nu_D(x) \rangle\, e^{\frac{-|z|^2}{4}} dz = 1 \qquad \text{for every } \; x \in \mathcal{F}D.$$

Indeed, by rotational invariance we may assume $H_{\nu_D(x)} = \mathbb{R}^{n-1} \times (0,\infty)$ and $\nu_D = e_n$, so

$$\int\limits_{H_{\nu_D(x)}} \langle z, \nu_D(x)\rangle\, e^{\frac{-|z|^2}{4}}\, dz \;=\; \int_{\mathbb{R}^{n-1}} e^{\frac{-|\tilde{z}|^2}{4}}\, d\tilde{z} \int_0^\infty z_n\, e^{\frac{-z_n^2}{4}}\, dz_n$$

$$= (4\pi)^{(n-1)/2} \cdot 2 = \frac{(4\pi)^{n/2}}{\sqrt{\pi}}.$$

□

Corollary 34. *Let $A, D \subset \mathbb{R}^n$ be two Caccioppoli sets satisfying $|A \setminus D| = 0$, then the equality*

$$\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_A\rangle = \mathcal{H}^{n-1}(\mathcal{F}A \cap \mathcal{F}D) \tag{2.29}$$

holds.

Proof: The fact $|A \setminus D| = 0$ implies that $\nu_A(x) = \nu_D(x)$ for $\mathcal{H}^{n-1}$-a.e. $x \in \mathcal{F}A \cap \mathcal{F}D$, so

$$\int\limits_{\mathcal{F}A\cap\mathcal{F}D} \langle \nu_A(x), \nu_D(x)\rangle\, d\mathcal{H}^{n-1}(x) = \mathcal{H}^{n-1}(\mathcal{F}A \cap \mathcal{F}D).$$

□

As a particular case, we take $A = D$ and obtain the following result which generalises M. Ledoux's result (see Chapter 1, Proposition 13) to an arbitrary Caccioppoli set in $\mathbb{R}^n$.

Theorem 35. *For a Caccioppoli set $D \subset \mathbb{R}^n$ the equality*

$$\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = P(D) \tag{2.30}$$

holds.

Proof: We take $A = D$ in (2.29) and obtain, since $P(D) = \mathcal{H}^{n-1}(\mathcal{F}D)$ and $\langle T(t)\mathbb{1}_D, \mathbb{1}_{\mathbb{R}^n}\rangle = \|T(t)\mathbb{1}_D\|_{L^1(\mathbb{R}^n)} = |D|$ for all $t \geq 0$, that

$$\begin{aligned}
P(D) &= \mathcal{H}^{n-1}(\mathcal{F}D) \\
&= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_D\rangle \\
&= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle \mathbb{1}_D - T(t)\mathbb{1}_D, \mathbb{1}_{\mathbb{R}^n} - \mathbb{1}_{D^c}\rangle \\
&= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \Big(\underbrace{\langle \mathbb{1}_D, \mathbb{1}_{\mathbb{R}^n}\rangle}_{=|D|} - \underbrace{\langle \mathbb{1}_D, \mathbb{1}_{D^c}\rangle}_{=0} - \underbrace{\langle T(t)\mathbb{1}_D, \mathbb{1}_{\mathbb{R}^n}\rangle}_{=|D|} + \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle \Big) \\
&= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle.
\end{aligned}$$

□

As a first consequence we obtain the following comparison principle for the evolution of the L^2-norm $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$.

Corollary 36. *Let $A, D \subset \mathbb{R}^n$ be two Caccioppoli sets of the same volume that satisfy the strict perimeter inequality $P(A) > P(D)$. Then there exists $t_1 > 0$ such that*

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2} \qquad \textit{for all } t \in (0, t_1).$$

Proof: By Theorem 35 we have that

$$\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = P(D).$$

Since the map $t \mapsto \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle$ is continuous on $(0,\infty)$, the strict inequality for the limits $P(A) > P(D)$ implies that there exists $\tilde{t_1} > 0$ such that

$$\frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c}\rangle > \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle \qquad \text{for all } t \in (0, \tilde{t_1})$$

and

$$\langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c}\rangle > \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle \qquad \text{for all } t \in (0, \tilde{t_1}). \tag{2.31}$$

By conservation of the total amount of heat in $\mathbb{R}^n$ we have

$$\begin{aligned} \langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c}\rangle + \langle T(t)\mathbb{1}_A, \mathbb{1}_A\rangle &= \langle T(t)\mathbb{1}_A, \mathbb{1}_{\mathbb{R}^n}\rangle = |A|, \\ \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle + \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle &= \langle T(t)\mathbb{1}_D, \mathbb{1}_{\mathbb{R}^n}\rangle = |D|. \end{aligned}$$

Since $|A| = |D|$ and (2.31) holds, it follows that

$$\langle T(t)\mathbb{1}_A, \mathbb{1}_A\rangle < \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle \qquad \text{for all } t \in (0, \tilde{t_1}). \tag{2.32}$$

In addition, we have (see Chapter 1, Section 1.1)

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2,$$

so (2.32) yields

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2} \qquad \text{for all } t \in (0, T) \text{ with } t_1 := 2\,\tilde{t_1}.$$

□

On the other hand we also obtain a corollary concerning the opposite implication.

Corollary 37. *Let $A, D \subset \mathbb{R}^n$ be two Caccioppoli sets of the same volume that satisfy an L^2-inequality*

$$\|T(t)\mathbb{1}_A\|_{L^2} \leq \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \in (0, t_1), \tag{2.33}$$

for some $t_1 > 0$. Then $P(A) \geq P(D)$.

Proof: By the same arguments as above the inequality (2.33) is equivalent to

$$\frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_A, \mathbb{1}_{A^c}\rangle \geq \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle, \qquad t \in (0, t_1).$$

Taking the limits as $t \to 0$ we obtain $P(A) \geq P(D)$. □

Chapter 3

Diffusion of characteristic functions: Long time behaviour

Motivation: Diffusion with Dirichlet boundary conditions

We motivate this chapter by recalling the long time behaviour of the diffusion of the characteristic function $\mathbb{1}_E$ of some bounded open set $E \subset \mathbb{R}^n$ in case we impose (vanishing) Dirichlet boundary conditions on ∂E. More precisely, we look at the long time behaviour of the following diffusion equation on $L^2(E)$

$$\text{(DHE)} \qquad \begin{cases} \frac{d}{dt}u(x,t) = \Delta_E^{\mathcal{D}} u(x,t), & t \geq 0, x \in E, \\ u(x,0) = \mathbb{1}_E(x), \end{cases}$$

where we denote by $\Delta_E^{\mathcal{D}}$ the *Dirichlet Laplacian* on $L^2(E)$ with domain

$$D(\Delta_E^{\mathcal{D}}) = \{f \in W_0^{1,2}(E) : \exists\, g \in L^2(E) \text{ such that } \Delta_E^{\mathcal{D}} f = g \text{ weakly}\}.$$

The semigroup $(T_E^{\mathcal{D}}(t))_{t\geq 0}$ yielding the solution of (DHE) is then given by an integral kernel $p_E^{\mathcal{D}}(x,y,t)$, the *Dirichlet heat kernel* of E. So the solution $T_E^{\mathcal{D}}(t)\mathbb{1}_E$ of (DHE) takes the form

$$T_E^{\mathcal{D}}(t)\mathbb{1}_E(x) = \int_E p_E^{\mathcal{D}}(x,y,t)\, \mathbb{1}_E(y)\, dy = \int_E p_E^{\mathcal{D}}(x,y,t)\, dy, \qquad x \in E, t > 0.$$

In this situation it is known (see e.g. [EN00, Chapter V]) that the long time behaviour of the solution is determined by the spectral bound of $\Delta_E^{\mathcal{D}}$, i.e., by the first (largest) Dirichlet eigenvalue $\lambda_1(E)$ since

$$s(\Delta_E^{\mathcal{D}}) = \sup\{\text{Re}\, \lambda : \lambda \in \sigma(\Delta_E^{\mathcal{D}})\} = \lambda_1(E) < 0.$$

Physically speaking, $-\lambda_1(E)$ is the fundamental frequency of E.
Since the semigroup $(T_E^{\mathcal{D}}(t))_{t\geq 0}$ is self-adjoint, it follows from the spectral theorem (see e.g. [EN00, Chapter I]) that

$$\|T_E^{\mathcal{D}}(t)\| \leq e^{t\lambda_1(E)}.$$

In particular, the total amount of heat that is still inside E after time $t > 0$, i.e., the quantity given by the inner product

$$\langle T_E^{\mathcal{D}}(t)\mathbb{1}_E, \mathbb{1}_E\rangle_{L^2(E)} = \int_E T_E^{\mathcal{D}}(t)\mathbb{1}_E(x)\,dx = \int_E\int_E p_E^{\mathcal{D}}(x,y,t)\,dy\,dx,$$

converges to zero with exponential rate $e^{t\lambda_1(E)}$ as $t \to \infty$.

Since for diffusion with Dirichlet boundary conditions the boundary has to be kept at temperature zero for all times $t > 0$, the diffusion process will, intuitively speaking, "never forget the geometry of the boundary". So it is quite reasonable that a quantity like $\lambda_1(E)$ which reflects information on the shape of the boundary determines the qualitative behaviour of the flow for large times.

In order to illustrate the significance of this geometric/physical condition we look at the following example of a Euclidean ball B and a ball D with a thin but long cut such that both B and D have the same volume.

Figure 3.1: Euclidean ball B and ball D with cut.

It is quite plausible that for large times the amount of heat still contained in D will decrease much faster than the amount of heat in B since the geometry of the boundary, here in particular the cut in the set D, has to be respected for all times.

Note that also for this kind of diffusion the ball B is extremal, i.e., keeps the heat for large times better than any other set: Under all sets having a given volume the ball has the largest first Dirichlet eigenvalue $\lambda_1(B)$ or, physically speaking, the lowest fundamental frequency. This is well known as the so called Faber-Krahn inequality for the first Dirichlet eigenvalues (see e.g. [Cha01], [Fab23], [Kra25]).

"Free" diffusion into the complement

In contrast to the situation described above, we now take the heat semigroup $(T(t))_{t\geq 0}$ on $L^2(\mathbb{R}^n)$, a compact set $D \subset \mathbb{R}^n$ and study the long time behaviour of the evolution

$$t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \geq 0.$$

This has been introduced in Chapter 1, Section 1.1 and treated in detail for small times in Chapter 2.

The physical significance is again that we consider the heat flow starting from the characteristic function of a compact set D without boundary condition on ∂D. Therefore we allow "free" heat flow out of D into the complement D^c. Since this "free" diffusion is a diffusion problem on the whole of $\mathbb{R}^n$, the spectral bound of the Laplacian Δ on $L^2(\mathbb{R}^n)$ is not less than 0 anymore. However, we have an explicit representation of the kernel which we will use constantly.

This representation implies immediately that

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle_{L^2(\mathbb{R}^n)} = \frac{1}{(4\pi t)^{n/2}} \int\limits_D \int\limits_D e^{\frac{-|x-y|^2}{4t}}\, dx\, dy$$

converges only polynomially to zero as $t \to \infty$.

Recall that in Chapter 1, Section 1.2 we deduced from the Riesz-Sobolev inequality the strict L^2-diffusion inequality

$$\|T(t)\mathbb{1}_D\|_{L^2} < \|T(t)\mathbb{1}_B\|_{L^2}, \qquad t > 0, \tag{3.1}$$

for a Euclidean ball B and some other compact set D of the same volume (which is not a ball). It states in particular that the characteristic function of a Euclidean ball B has the optimal diffusion property for *large* times.

We now want to identify the reason why the ball has this extremal property with respect to *large* times. This is important if one wants to compare the corresponding evolutions for two arbitrary compact sets and not just for the ball and a second set like in (3.1). The main problem clearly is that Euclidean balls are extremal with respect to so many properties that it is difficult to identify the one that causes the phenomenon under consideration. For a nice overview over many extremal properties of the ball, see [PS51].

As a main result of the previous chapter (Chapter 2, Corollary 36) we proved a partial generalisation of (3.1) for *small* times stating that for two arbitrary compact sets $A, D \subset \mathbb{R}^n$ of the same volume the implication

$$P(A) > P(D) \qquad \Longrightarrow \qquad \|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \in (0, t_1), \tag{3.2}$$

holds with some $t_1 \in (0, \infty]$. It is possible to have $t_1 = \infty$, but in general the inequality for the L^2-norms will hold only on a finite, possibly very small time interval.

The aim now is to find the "large time analogue" to implication (3.2). As a first result in this direction we will show (Proposition 43) that for two arbitrary compact sets A, D of the same volume we have

$$\int_A \int_A |x-y|^2 \, dx \, dy > \int_D \int_D |x-y|^2 \, dx \, dy \Rightarrow \|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2}, \; t \in (t_2, \infty) \quad (3.3)$$

for some $t_2 \in [0, \infty)$. Afterwards we will further describe the integrals on the left hand side by physical quantities of the sets A and D - considered as rigid bodies - like momenta and inertial tensors (Proposition 47 and 51).

The results we are going to establish can be coined, in the two-dimensional situation, into the following rule of thumb: *If two compact sets of the same volume are fixed in their center of gravity, and both are given the same angular momentum, then the one which turns faster will keep the heat better for large times.*

As an introductory example we will discuss a special situation where we can prove explicitly a strict L^2-diffusion inequality not only for large, but even for all positive times.

3.1 Heat diffusion for ring domains

We look at the following class of compact sets in $\mathbb{R}^n$.

Definition 38. Given two Euclidean balls $B_1, B_2 \subset \mathbb{R}^n$ such that $B_1 \subset B_2$. We call the set $D := B_2 \setminus B_1$ a *ring domain* in $\mathbb{R}^n$ obtained from the balls B_1 and B_2.

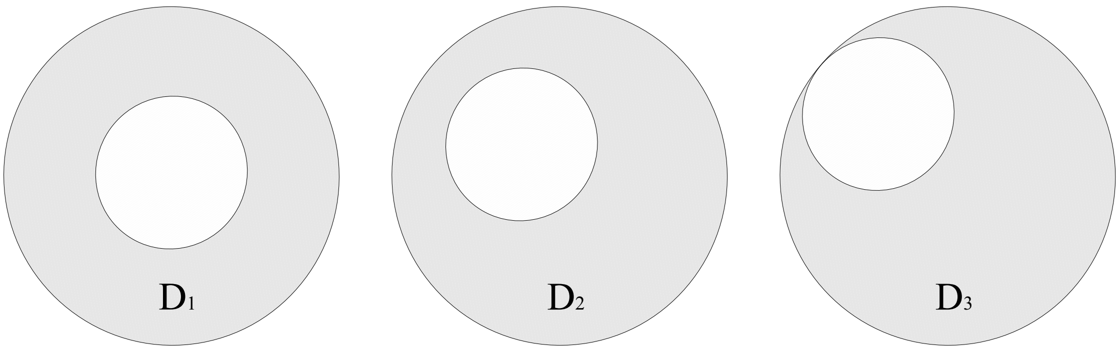

Figure 3.2: Ring domains in $\mathbb{R}^2$.

For the diffusion of characteristic functions of ring domains we prove the following comparison result.

Proposition 39 (Diffusion for ring domains). *Given a Euclidean ball $B \subset \mathbb{R}^n$ and three smaller balls $C_1, C_2, C_3 \subset B$ with $|C_1| = |C_2| = |C_3|$ such that C_1 has the same center as B, C_3 touches the boundary of B and C_2 lies somewhere in between (as drawn in Figure 3.2). Further denote by $D_1 := B \setminus C_1, D_2 := B \setminus C_2, D_3 := B \setminus C_3$ the corresponding ring domains. Then*

$$\|T(t)\mathbb{1}_{D_1}\|_{L^2} < \|T(t)\mathbb{1}_{D_2}\|_{L^2} < \|T(t)\mathbb{1}_{D_3}\|_{L^2}, \qquad t > 0. \quad (3.4)$$

Remark 40. The above proposition in particular says that a ring domain keeps the heat the better the more it is asymmetric. This corresponds to the statement from above that the "more concentrated" the volume of a set is, the better the heat will be kept inside the set at least for large times.

For the proof we need the following elementary facts on the diffusion of characteristic functions of Euclidean balls.

Lemma 41. *Let $B \subset \mathbb{R}^n$ be a Euclidean ball centered in the origin. For every $t > 0$ the function*

$$T(t)\mathbb{1}_B(x) = \frac{1}{(4\pi t)^{n/2}} \int_B e^{\frac{-|x-y|^2}{4t}}\, dy, \qquad x \in \mathbb{R}^n,$$

is positive, radially symmetric with respect to the origin and strictly decreasing as $|x|$ increases, i.e.,

$$\begin{aligned} T(t)\mathbb{1}_B(x) &= T(t)\mathbb{1}_B(\tilde{x}), && |x| = |\tilde{x}|, \\ \textit{and} \quad T(t)\mathbb{1}_B(x) &> T(t)\mathbb{1}_B(\tilde{x}), && |x| < |\tilde{x}|. \end{aligned}$$

Proof: The positivity is immediate by the positivity of the kernel. The radial symmetry follows from the fact that the kernel as well as the ball B are symmetric. Finally $T(t)\mathbb{1}_B$ is strictly decreasing as $|x| \to \infty$ since the exponential function contained in the kernel is strictly decreasing. □

Proof of the proposition: From Section 1.1 we have the relation

$$\|T(\tfrac{t}{2})\mathbb{1}_{D_i}\|_{L^2}^2 = \langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle.$$

So it is enough to prove that

$$\langle T(t)\mathbb{1}_{D_1}, \mathbb{1}_{D_1}\rangle < \langle T(t)\mathbb{1}_{D_2}, \mathbb{1}_{D_2}\rangle < \langle T(t)\mathbb{1}_{D_3}, \mathbb{1}_{D_3}\rangle, \qquad t > 0.$$

Since $\mathbb{1}_{D_i} = \mathbb{1}_B - \mathbb{1}_{C_i}$, we write $\langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle$ in the following way:

$$\begin{aligned} \langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle &= \langle T(t)(\mathbb{1}_B - \mathbb{1}_{C_i}), \mathbb{1}_B - \mathbb{1}_{C_i}\rangle \\ &= \langle T(t)\mathbb{1}_B - T(t)\mathbb{1}_{C_i}, \mathbb{1}_B - \mathbb{1}_{C_i}\rangle \\ &= \langle T(t)\mathbb{1}_B, \mathbb{1}_B - \mathbb{1}_{C_i}\rangle - \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_B - \mathbb{1}_{C_i}\rangle \\ &= \langle T(t)\mathbb{1}_B, \mathbb{1}_B\rangle - \langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle - \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_B\rangle + \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_{C_i}\rangle. \end{aligned}$$

Again by the symmetry of $T(t)$ the summands $\langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle$ and $\langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_B\rangle$ coincide. Therefore

$$\begin{aligned} \langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle &= \langle T(t)\mathbb{1}_B, \mathbb{1}_B\rangle - \langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle - \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_B\rangle + \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_{C_i}\rangle \\ &= \langle T(t)\mathbb{1}_B, \mathbb{1}_B\rangle - 2\langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle + \langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_{C_i}\rangle. \end{aligned}$$

Next, since the heat equation is invariant under translations of $\mathbb{R}^n$, the product $\langle T(t)\mathbb{1}_{C_i}, \mathbb{1}_{C_i}\rangle$, and clearly also $\langle T(t)\mathbb{1}_B, \mathbb{1}_B\rangle$, are independent of the position of C_i and B. Therefore, in order to minimize the product $\langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle$, i.e., to minimize the amount of heat still contained inside of D_i after an arbitrary time $t > 0$, we have to choose the C_i such that $\langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle$ becomes maximal.

Since by Lemma 41 the function $T(t)\mathbb{1}_B$ is positive, rotationally symmetric and strictly decreasing with respect to its center, one has to locate C_i in the center of B to maximize $\langle T(t)\mathbb{1}_B, \mathbb{1}_{C_i}\rangle$ and therefore to minimize $\langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle$. The more we move C_i away the larger $\langle T(t)\mathbb{1}_{D_i}, \mathbb{1}_{D_i}\rangle$ becomes and it is maximal if ∂C_i touches the boundary of B. □

Remark 42. This special class of sets is interesting also from a different perspective: In case we have equality of perimeters, $P(A) = P(D)$, we can not apply (3.2) from above and the example shows that it is in general not possible to make any assertion about the relation of the L^2-norms $\|T(t)\mathbb{1}_A\|_{L^2}$ and $\|T(t)\mathbb{1}_D\|_{L^2}$ for small $t > 0$.

After this introductory example we now study the general situation for the long time behaviour of the flow $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$ for arbitrary compact subsets of the same volume.

3.2 Heat diffusion for arbitrary compact sets

The following result shows the main connections between integrals describing the "distribution of volume" for given compact sets $A, D \subset \mathbb{R}^n$ and the long time behaviour for the diffusion of their characteristic functions, as mentioned above in (3.3).

Note that in the whole section we will need no smoothness assumptions on the boundaries of the regarded sets.

Proposition 43 (Long time diffusion behaviour). *Let $A, D \subset \mathbb{R}^n$ be two compact sets of the same volume that satisfy a strict inequality*

$$\int_A \int_A |x-y|^2 \, dx \, dy > \int_D \int_D |x-y|^2 \, dx \, dy. \tag{3.5}$$

Then there exists $t_2 \in [0, \infty)$ such that

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t > t_2. \tag{3.6}$$

In case we have equality for the integrals in (3.5) but a strict (opposite!) inequality for the integrals over the fourth powers of the distances, i.e.,

$$\int_A \int_A |x-y|^4 \, dx \, dy < \int_D \int_D |x-y|^4 \, dx \, dy, \tag{3.7}$$

then the same conclusion (3.6) holds.
In general the integrals with the smallest exponent $2n$ such that the integrals

$$\int_A \int_A |x-y|^{2n} \, dx \, dy \qquad \text{and} \qquad \int_D \int_D |x-y|^{2n} \, dx \, dy$$

are not equal, e.g., without loss of generality

$$(-1)^n \int_A \int_A |x-y|^{2n}\,dx\,dy < (-1)^n \int_D \int_D |x-y|^{2n}\,dx\,dy, \tag{3.8}$$

*determine the long time behaviour (*3.6*).*

Proof: For a compact set $A \subset \mathbb{R}^n$ we first define the following function

$$\varphi_A(\tau) := \int_A \int_A e^{-\tau|x-y|^2}\,dx\,dy, \qquad \tau \in \mathbb{R}.$$

Since

$$\varphi_A(0) = \int_A \int_A dx\,dy = |A|^2,$$

we conclude

$$\varphi_A(0) = \varphi_D(0). \tag{3.9}$$

From the definition it is clear that $\varphi_A \in C^\infty(\mathbb{R})$. Since A is compact, we obtain the derivatives of $\varphi_A(\tau)$ by differentiating under the integral sign

$$\begin{aligned} \frac{d}{d\tau}\varphi_A(\tau) &= -\int_A \int_A |x-y|^2 e^{-\tau|x-y|^2}\,dx\,dy, \\ \frac{d^2}{d\tau^2}\varphi_A(\tau) &= \int_A \int_A |x-y|^4 e^{-\tau|x-y|^2}\,dx\,dy \\ \text{and} \quad \frac{d^n}{d\tau^n}\varphi_A(\tau) &= (-1)^n \int_A \int_A |x-y|^{2n} e^{-\tau|x-y|^2}\,dx\,dy. \end{aligned}$$

So we have at $\tau = 0$:

$$\begin{aligned} \frac{d}{d\tau}\varphi_A(0) &= -\int_A \int_A |x-y|^2\,dx\,dy, \\ \frac{d^2}{d\tau^2}\varphi_A(0) &= \int_A \int_A |x-y|^4\,dx\,dy \\ \text{and} \quad \frac{d^n}{d\tau^n}\varphi_A(0) &= (-1)^n \int_A \int_A |x-y|^{2n}\,dx\,dy. \end{aligned}$$

Therefore, in case of condition (3.5), i.e.,

$$\int_A \int_A |x-y|^2\,dx\,dy > \int_D \int_D |x-y|^2\,dx\,dy$$

this means that

$$\frac{d}{d\tau}\varphi_A(0) < \frac{d}{d\tau}\varphi_D(0). \tag{3.10}$$

In case conditions (3.7) are satisfied we can write

$$\frac{d}{d\tau}\varphi_A(0) = \frac{d}{d\tau}\varphi_D(0) \quad \text{and} \quad \frac{d^2}{d\tau^2}\varphi_A(0) < \frac{d^2}{d\tau^2}\varphi_D(0), \tag{3.11}$$

and in the general situation (3.8) we have

$$\frac{d^k}{d\tau^k}\varphi_A(0) = \frac{d^k}{d\tau^k}\varphi_D(0),\ k=1,...,n-1 \quad \text{and} \quad \frac{d^n}{d\tau^n}\varphi_A(0) < \frac{d^n}{d\tau^n}\varphi_D(0). \tag{3.12}$$

Now, each of these cases together with the equality (3.9) imply by using the Taylor expansion for the functions φ_A and φ_D near zero that there exists $\tilde{t}_2 \in (0,\infty]$ such that

$$\varphi_A(\tau) < \varphi_D(\tau), \qquad \tau \in (0,\tilde{t}_2),$$

i.e.,

$$\int_A\int_A e^{-\tau|x-y|^2}\,dx\,dy < \int_D\int_D e^{-\tau|x-y|^2}\,dx\,dy, \qquad \tau \in (0,\tilde{t}_2).$$

After the substitution $t := \frac{1}{4\tau}$ and multiplication with $\frac{1}{(4\pi t)^{n/2}} > 0$ we obtain

$$\frac{1}{(4\pi t)^{n/2}}\int_A\int_A e^{\frac{-|x-y|^2}{4t}}\,dy\,dx < \frac{1}{(4\pi t)^{n/2}}\int_D\int_D e^{\frac{-|x-y|^2}{4t}}\,dy\,dx, \quad t \in \Big(\frac{1}{4\,\tilde{t}_2},\infty\Big), \tag{3.13}$$

which in case $\tilde{t}_2 = \infty$ holds for all $t \in (0,\infty)$. Using the identity

$$\frac{1}{(4\pi t)^{n/2}}\int_A\int_A e^{\frac{-|x-y|^2}{4t}}\,dy\,dx = \langle T(t)\mathbb{1}_A, \mathbb{1}_A\rangle = \|T(\tfrac{t}{2})\mathbb{1}_A\|^2_{L^2},$$

we rewrite (3.13) as

$$\|T(\tfrac{t}{2})\mathbb{1}_A\|^2_{L^2} < \|T(\tfrac{t}{2})\mathbb{1}_D\|^2_{L^2}, \qquad t \in \Big(\tfrac{1}{4\,\tilde{t}_2},\infty\Big).$$

So we finally have

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \in (t_2,\infty), \quad t_2 := \frac{1}{8\,\tilde{t}_2},$$

which in case $\tilde{t}_2 = \infty$ holds for all $t \in (0,\infty)$. □

However, for applications and in order to determine explicitly the integrals in (3.5) and (3.7) it will be interesting to find relations between these integrals and physical quantities of the sets under consideration - considered as rigid bodies.

We will make use of the concept of moments coming from physics, which plays an important role, e.g., in the multipole expansions in electrostatics and in the theory of rigid bodies. There, not only the total amout of charges or the total mass is important, but also their distribution throughout the field or the body, for which the moments yield an appropriate description.

Therefore we continue with the following definitions.

Definition 44. Let $D \subset \mathbb{R}^n$ be a compact set. We denote by $\overline{x}_D$ its *center of gravity*

$$\overline{x}_D := \frac{1}{|D|} \int\limits_D x \, dx.$$

Further, we define by

$$\mu_2(D) := \frac{1}{|D|} \int\limits_D |x - \overline{x}_D|^2 \, dx$$

the *second central moment of* D, i.e., the second moment with respect to the center of gravity $\overline{x}_D$. The *fourth central moment of* D is

$$\mu_4(D) := \frac{1}{|D|} \int\limits_D |x - \overline{x}_D|^4 \, dx.$$

Definition 45. Let $D \subset \mathbb{R}^n$ be a compact set. We define the *inertia tensor* $\Theta^D := (\Theta^D_{ij})_{1 \le i,j \le n}$ of D with respect to the origin by

$$\Theta^D_{ij} := \int\limits_D x_i x_j \, dx,$$

and recall that the Hilbert-Schmidt norm of the tensor Θ^D is given by

$$\|\Theta^D\|_{HS} = \Big(\sum_{ij} (\Theta^D_{ij})^2 \Big)^{1/2}.$$

Remark 46. Note that if D has center of gravity in the origin, then the *second central moment* $\mu_2(D)$ *of* D is - up to the volume $|D|$ - equal to the *trace* $\mathrm{tr}\,(\Theta^D)$ *of the inertial tensor* Θ^D:

$$\mu_2(D) = \frac{1}{|D|} \int\limits_D |x|^2 \, dx = \frac{1}{|D|} \sum_{i=1}^n \int\limits_D x_i^2 \, dx = \frac{1}{|D|} \sum_{i=1}^n \Theta^D_{ii} = \frac{1}{|D|} \mathrm{tr}\,(\Theta^D).$$

Now we will connect the integrals

$$\int\limits_D \int\limits_D |x - y|^2 \, dx \, dy \quad \text{and} \quad \int\limits_D \int\limits_D |x - y|^4 \, dx \, dy,$$

with the quantities defined above and start with the integral of the squared distances.

3.2.1 The quantity $\int\limits_D \int\limits_D |x-y|^2 \, dx \, dy$

We first show that the integral over the squared distances in $D \times D$ is up to a constant the second central moment $\mu_2(D)$ of D.

Proposition 47. *Let $D \subset \mathbb{R}^n$ be a compact set, $\overline{x}_D$ its center of gravity. Then it holds that*

$$\int\limits_D \int\limits_D |x-y|^2 \, dx \, dy \; = \; 2\,|D| \int\limits_D |x-\overline{x}_D|^2 \, dx \; = \; 2\,|D|^2 \, \mu_2(D). \tag{3.14}$$

In particular, for two compact sets $A, D \subset \mathbb{R}^n$ of the same volume $|A| = |D|$ the equivalence

$$\mu_2(A) \leq \mu_2(D) \quad \Longleftrightarrow \quad \int\limits_A \int\limits_A |x-y|^2 \, dx \, dy \leq \int\limits_D \int\limits_D |x-y|^2 \, dx \, dy$$

holds.

Proof: The second equality in (3.14) follows directly by definition of the second central moment $\mu_2(D)$.
In order to prove the first equality we denote by $D_0 := D - \overline{x}_D$ the translation of D which has its center of gravity in the origin. Since the integral $\int\limits_D \int\limits_D |x-y|^2 \, dx \, dy$ is invariant under translation of D we obtain by polarisation that

$$\begin{aligned}
\int\limits_D \int\limits_D |x-y|^2 \, dx \, dy \;&=\; \int\limits_{D_0} \int\limits_{D_0} |x-y|^2 \, dx \, dy \\
&=\; \int\limits_{D_0} \int\limits_{D_0} \langle x-y, x-y \rangle \, dx \, dy \\
&=\; \int\limits_{D_0} \int\limits_{D_0} \Big(|x|^2 + |y|^2 - 2\langle x, y \rangle \Big) \, dx \, dy \\
&=\; \int\limits_{D_0} \int\limits_{D_0} |x|^2 \, dx \, dy + \int\limits_{D_0} \int\limits_{D_0} |y|^2 \, dx \, dy - 2 \int\limits_{D_0} \int\limits_{D_0} \langle x, y \rangle \, dx \, dy \\
&=\; |D_0| \int\limits_{D_0} |x|^2 \, dx + |D_0| \int\limits_{D_0} |y|^2 \, dy - 2 \int\limits_{D_0} \int\limits_{D_0} \langle x, y \rangle \, dx \, dy \\
&=\; 2\,|D_0| \int\limits_{D_0} |x|^2 \, dx - 2 \int\limits_{D_0} \int\limits_{D_0} \langle x, y \rangle \, dx \, dy \\
&=\; 2\,|D_0| \int\limits_{D_0} |x|^2 \, dx - 2 \Big\langle \underbrace{\int\limits_{D_0} y \, dy}_{=0}, \underbrace{\int\limits_{D_0} x \, dx}_{=0} \Big\rangle \\
&=\; 2\,|D_0| \int\limits_{D_0} |x|^2 \, dx,
\end{aligned}$$

since the center of gravity $\overline{x}_{D_0}$ of D_0 coincides with the origin and clearly $|D_0| = |D|$. Since

$$\int_{D_0} |x|^2\, dx = \int_{D} |x - \overline{x}_D|^2\, dx,$$

we obtain the desired equality

$$\begin{aligned} \int_D \int_D |x-y|^2\, dx\, dy &= 2\,|D_0| \int_{D_0} |x|^2\, dx \\ &= 2\,|D| \int_D |x - \overline{x}_D|^2\, dx. \quad \square \end{aligned}$$

Therefore, in order to minimize the integral

$$\int_D \int_D |x-y|^2\, dx\, dy$$

under all compact sets of a given volume, we can instead minimize the second central moment $\mu_2(D)$ of D. As an easy consequence we obtain the following corollary.

Corollary 48. *The following assertions hold true.*
i) Under all compact sets $D \subset \mathbb{R}^n$ of the same volume the Euclidean ball $D = B$ minimizes the integral

$$\int_D \int_D |x-y|^2\, dx\, dy. \tag{3.15}$$

ii) Further, for every compact set $D \subset \mathbb{R}^n$ it holds that

$$\frac{\mu_2(D)}{|D|} \geq \frac{n}{(n+2)\,\omega_n\, R^{n-2}}, \tag{3.16}$$

where $\omega_n = |\mathbb{B}^n|$ is the volume of the n-dimensional unit ball and R is the radius of the Euclidean ball B_R having the same volume as D, i.e., $R = \left(\frac{|D|}{\omega_n}\right)^{1/n}$. Equality in (3.16) is attained if D is a Euclidean ball.

Remark 49. The assertion of the corollary should be compared with the "isoperimetric property" of the ball: This time one does not compare volume and perimeters which was the crucial relation for the short time behaviour of the flow, but volume and second central moments.

Proof: i) By Proposition 47 we only have to show that for a given volume the Euclidean ball of this volume minimizes the integral

$$\int_D |x - \overline{x}_D|^2\, dx = \int_{D_0} |x|^2\, dx.$$

Since $x \mapsto |x|^2$ is a positive, monotone, radially symmetric function having its minimum in the origin, the integral is minimized if and only if the integration domain is the Euclidean ball B with center in the origin.
ii) By i) the Euclidean ball $B \subset \mathbb{R}^n$ minimizes the integral (3.15) and therefore the second central moment under all compact sets of the same volume. So B minimizes the quotient $\frac{\mu_2(D)}{|D|}$, and we obtain

$$\begin{aligned}\frac{\mu_2(B_R)}{|B_R|} &= \frac{1}{|B_R|^2}\int_{B_R}|x|^2\,dx = \frac{1}{(\omega_n R^n)^2}\int_{S^{n-1}}\int_0^R r^{n-1}|r\omega|^2\,d\omega\,dr \\ &= \frac{|S^{n-1}|}{(\omega_n R^n)^2}\int_0^R r^{n+1}\,dr = \frac{n\,\omega_n}{(\omega_n R^n)^2}\cdot\frac{R^{n+2}}{n+2} \\ &= \frac{n}{(n+2)\,\omega_n\,R^{n-2}}. \quad \square\end{aligned}$$

Remark 50. Now, independently of the L^2-diffusion inequality (Chapter 1, Theorem 7) which compares Euclidean balls with other compact sets of the same volume, we obtain that for *large* times a Euclidean ball keeps heat better than any other set of the same volume.
But this time, we can even compare the large time heat diffusion of the characteristic functions of two arbitrary compact sets $A, D \subset \mathbb{R}^n$ of the same volume.

We next come to the situation where the second central moments are equal. Here the integrals of the fourth power of the distances decide about the comparison of the norms $\|T(t)\mathbb{1}_A\|_{L^2}$ and $\|T(t)\mathbb{1}_D\|_{L^2}$ for large times.

3.2.2 The quantity $\int_D\int_D |x-y|^4\,dx\,dy$

Here the situation is not as nice as before, but at least we obtain the following connections.

Proposition 51. *Let $D \subset \mathbb{R}^n$ be a compact set with center of gravity $\overline{x}_D$ in the origin. Then we have the following decomposition*

$$\int_D\int_D |x-y|^4\,dx\,dy = 2\,|D|\int_D |x|^4 + 2\Big(\int_D |x|^2\,dx\Big)^2 + 4\int_D\int_D \langle x,y\rangle^2\,dx\,dy \quad (3.17)$$

$$= 2\,|D|^2\,\mu_4(D) + 2[|D|\,\mu_2(D)]^2 + 4\,\|\Theta^D\|_{HS}^2. \quad (3.18)$$

In particular, for two compact subsets $A, D \subset \mathbb{R}^n$ with $|A| = |D|$ and $\mu_2(A) = \mu_2(D)$ the following implication holds

$$\left.\begin{array}{rcl}\mu_4(A) &<& \mu_4(D)\\ \|\Theta^A\|_{HS} &\le& \|\Theta^D\|_{HS}\end{array}\right\} \implies \int_A\int_A |x-y|^4\,dx\,dy < \int_D\int_D |x-y|^4\,dx\,dy.$$

Proof: At first we have the following decomposition

$$\begin{aligned}
\int_D\int_D |x-y|^4\,dx\,dy &= \int_D\int_D \langle x-y, x-y\rangle^2\,dx\,dy \\
&= \int_D\int_D (|x|^2 - 2\,\langle x,y\rangle + |y|^2)^2\,dx\,dy \\
&= \int_D\int_D |x|^4 - 2\langle x,y\rangle|x|^2 + |x|^2|y|^2\,dx\,dy \\
&\quad + \int_D\int_D -2\langle x,y\rangle|x|^2 + 4\langle x,y\rangle^2 - 2\langle x,y\rangle|y|^2\,dx\,dy \\
&\quad + \int_D\int_D |y|^4 - 2\langle x,y\rangle|y|^2 + |x|^2|y|^2\,dx\,dy \\
&= 2\int_D\int_D |x|^4\,dx\,dy + 2\int_D\int_D |x|^2|y|^2\,dx\,dy \\
&\quad + 4\int_D\int_D \langle x,y\rangle^2\,dx\,dy - 8\int_D\int_D \langle x,y\rangle|x|^2\,dx\,dy.
\end{aligned}$$

Since

$$\int_D\int_D \langle x,y\rangle|x|^2\,dx\,dy = \int_D\int_D \langle x|x|^2, y\rangle\,dx\,dy = \langle \int_D x|x|^2\,dx, \underbrace{\int_D y\,dy\rangle}_{=0} = 0,$$

we obtain (3.17)

$$\int_D\int_D |x-y|^4\,dx\,dy = 2\,|D|\int_D |x|^4\,dx + 2\Big(\int_D |x|^2\,dx\Big)^2 + 4\int_D\int_D \langle x,y\rangle^2\,dx\,dy.$$

Now note that by

$$\begin{aligned}
\int_D\int_D \langle x,y\rangle^2\,dx\,dy &= \int_D\int_D \Big(\sum_{i=1}^n x_i y_i\Big)^2\,dx\,dy = \sum_{i,j=1}^n \int_D\int_D x_i x_j y_i y_j\,dx\,dy \\
&= \sum_{i,j=1}^n \Big(\int_D x_i x_j\,dx\Big)^2 = \sum_{i,j=1}^n (\Theta_{ij}^D)^2 \\
&= \|\Theta^D\|_{HS}^2
\end{aligned}$$

the integral $\int_D\int_D \langle x,y\rangle^2\,dx\,dy$ gives the squared Hilbert-Schmidt norm of the tensor Θ^D.

So we altogether obtain

$$\int_D\int_D |x-y|^4\,dx\,dy = 2\,|D|\int_D |x|^4\,dx + 2\Big(\int_D |x|^2\,dx\Big)^2 + 4\int_D\int_D \langle x,y\rangle^2\,dx\,dy$$

and therefore (3.18)

$$\int_D \int_D |x-y|^4 \, dx \, dy = 2\,|D|^2\,\mu_4(D) + 2[|D|\,\mu_2(D)]^2 + 4\,\|\Theta^D\|_{HS}^2$$

by definition of the second and fourth central moments of D. □

We summarize the main results in the following theorem.

Theorem 52 (Long time behaviour). *Let $A, D \subset \mathbb{R}^n$ be two compact sets of the same volume $|A| = |D|$ that satisfy the strict inequality*

$$\mu_2(A) > \mu_2(D) \tag{3.19}$$

for the second central moments. Then there exists $t_2 \in [0, \infty)$ such that

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2} \qquad \text{for all } t > t_2. \tag{3.20}$$

In case we have equality in (3.19) and a strict (opposite!) inequality

$$\int_A \int_A |x-y|^4 \, dx \, dy < \int_D \int_D |x-y|^4 \, dx \, dy, \tag{3.21}$$

then the same conclusion (3.20) holds.
Furthermore, inequality (3.21) follows, e.g., if we have

$$\mu_4(A) < \mu_4(D) \quad \text{and} \quad \|\Theta^A\|_{HS} \le \|\Theta^D\|_{HS}$$

for the fourth central moments and the Hilbert-Schmidt norm of the inertial tensors Θ^A and Θ^D.

Remark 53. As we see from the L^2-diffusion inequality (see Section 1.2) for a ball and any other set of the same volume and in addition from the class of ring domains discussed in Section 3.1 it is possible to have $t_2 = 0$. In general t_2 will be strictly positive as the following example (Figure 3.3) should illustrate.

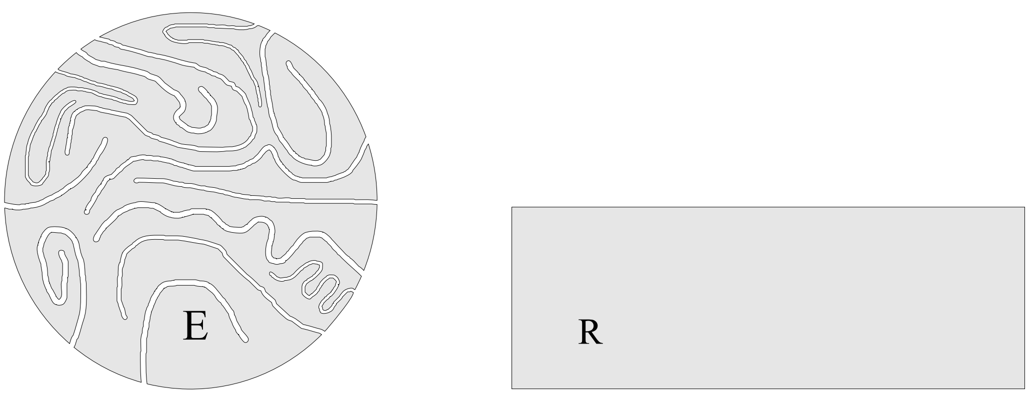

Figure 3.3: Ball E with cuts and rectangle R.

Example 54. We assume E and R have the same volume and are as in figure 3.3. It is immediate that the set E has larger perimeter than R, i.e., $P(E) > P(R)$. This implies that

$$\|T(t)\mathbb{1}_E\|_{L^2} < \|T(t)\mathbb{1}_R\|_{L^2} \qquad \text{for } \textit{small}\ t > 0.$$

On the other hand, R obviously has larger second central moment than E:

$$\int_E |x - \overline{x}_E|^2\, dx < \int_R |x - \overline{x}_R|^2\, dx.$$

So we have

$$\|T(t)\mathbb{1}_E\|_{L^2} > \|T(t)\mathbb{1}_R\|_{L^2}$$

for *large* values of t.

Obviously, in the notation used above, we can not have $t_1 = \infty$ or $t_2 = 0$ since the L^2-diffusion inequality has the opposite inequality sign for short and for large times, respectively. This means that the L^2-inequality has to "switch" at least once after a certain time.

However, even with the inequalities

$$P(A) > P(D) \qquad \text{and} \qquad \mu_2(A) > \mu_2(D)$$

for two compact sets $A, D \subset \mathbb{R}^n$ of the same volume, we only know that

$$\|T(t)\mathbb{1}_A\|_{L^2} < \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \in (0, t_1) \cup (t_2, \infty), \tag{3.22}$$

for some t_1, t_2.

It remains an open problem to find (maybe additional?) sufficient conditions on the sets A and D such that (3.22) holds for *all* times $t > 0$.

3.3 Examples

3.3.1 Examples (μ_2 - second central moment)

In order to illustrate the above results we look at the following examples of subsets of $\mathbb{R}^2$ and compare explicitly their second central moments.

i) Euclidean ball $B_R \subset \mathbb{R}^2$ with radius $R > 0$:

$$\begin{aligned}\mu_2(B_R) &= \frac{1}{|B_R|} \int_{B_R} |x|^2\, dx = \frac{1}{|B_R|} \int_{S^1} \int_0^R r|r\omega|^2\, d\omega\, dr \\ &= \frac{|S^1|}{|B_R|} \int_0^R r^3\, dr = \frac{2\pi}{R^2\pi} \frac{R^4}{4} = \frac{R^2}{2}.\end{aligned}$$

For $|B_R| = 1$, i.e., $R = \frac{1}{\sqrt{\pi}}$, we have $\mu_2(B_{\frac{1}{\sqrt{\pi}}}) = \frac{1}{2\pi} \approx 0,15915$.

ii) Square $S_a \subset \mathbb{R}^2$ with side length a:

$$\mu_2(S_a) = \frac{1}{|S_a|} \int_P |x|^2 \, dx = \frac{4}{a^2} \int_0^{\frac{a}{2}} \int_0^{\frac{a}{2}} x_1^2 + x_2^2 \, dx_1 \, dx_2 = \frac{4}{a^2} \cdot \frac{1}{24} a^4 = \frac{1}{6} a^2.$$

For $|S_a| = 1$, i.e., $a = 1$, we have $\mu_2(S_1) = \frac{1}{6} \approx 0,16667$.

iii) Parallelogram $P1 \subset \mathbb{R}^2$ bounded by $f(x) = -\frac{1}{2}|x| + \frac{1}{2}$ and $-f(x)$ with volume $|P1| = 1$:

$$\mu_2(P1) = \frac{1}{|P1|} \int_P |x|^2 \, dx = 4 \int_0^1 \int_0^{-\frac{1}{2}x_2 + \frac{1}{2}} x_1^2 + x_2^2 \; dx_1 \, dx_2 = 4 \cdot \frac{5}{96} = \frac{5}{24} \approx 0,20833.$$

iv) Parallelogram $P2 \subset \mathbb{R}^2$ bounded by $g(x) = -\frac{1}{8}|x| + \frac{1}{4}$ and $-g(x)$ with volume $|P2| = 1$:

$$\mu_2(P2) = \frac{1}{|P2|} \int_{P1} |x|^2 \, dx = 4 \int_0^2 \int_0^{-\frac{1}{8}x_2 + \frac{1}{4}} x_1^2 + x_2^2 \; dx_1 \, dx_2 = 4 \cdot \frac{65}{384} = \frac{65}{96} \approx 0,67708.$$

v) Family of rectangles $R_a \subset \mathbb{R}^2$ with side lengths a and $\frac{1}{a}$ with volume $|R_a| = 1$:

$$\mu_2(R_a) = \frac{1}{|R_a|} \int_R |x|^2 \, dx = 4 \int_0^{\frac{a}{2}} \int_0^{\frac{1}{2a}} x_1^2 + x_2^2 \, dx_1 \, dx_2 = 4 \cdot \frac{1}{48}(a^2 + \frac{1}{a^2}) = \frac{1}{12}(a^2 + \frac{1}{a^2}).$$

So we have the following table for second central moments which explicitly allows to compare the long time behaviour for the diffusion of the corresponding characteristic functions.

set	*volume*	μ_2
Euclidean ball	1	0,15915
square	1	0,16667
rectangle ($a = \frac{95}{100}$)	1	0,16754
rectangle ($a = \frac{9}{10}$)	1	0,17038
rectangle ($a = \frac{8}{10}$)	1	0,18354
parallelogram $P1$	1	0,20833
rectangle ($a = \frac{1}{2}$)	1	0,35417
parallelogram $P2$	1	0,67708
rectangle ($a = \frac{1}{5}$)	1	2,08667
rectangle ($a = \frac{1}{10}$)	1	8,33417
rectangle ($a = \frac{1}{20}$)	1	33,33354
rectangle ($a = \frac{1}{50}$)	1	208,33337
rectangle ($a = \frac{1}{100}$)	1	833,33333

3.3.2 Examples (μ_4 - fourth central moment)

Finally we give an example of two compact sets A, D in $\mathbb{R}^2$ having the same volume, the same second central moment, but different fourth central moments and satisfy the condition of Theorem 52 for the Hilbert-Schmidt norms of Θ^A and Θ^D.

We first consider the family of rectangles

$$R_a = [-4a, 4a] \times [-\frac{4}{a}, \frac{4}{a}], \qquad a > 0.$$

Then R_a has volume $|R_a| = 64$ (independently of a) and second central moment (depending on a)

$$\mu_2(R_a) = \frac{1}{|R_a|} \int\limits_{R_a} |x|^2 \, dx = \frac{4}{64} \int\limits_0^{4a} \int\limits_0^{\frac{4}{a}} x_1^2 + x_2^2 \, dx_1 \, dx_2 = \frac{16}{3} \frac{(a^4+1)}{a^2}.$$

Further we take the family of parallelograms P_a bounded by the functions f_a and $-f_a$ which are given by

$$f_a(x) := \begin{cases} \frac{8}{a^2}x + \frac{16}{a}, & x < 0, \\ -\frac{8}{a^2}x + \frac{16}{a}, & x \geq 0. \end{cases}$$

Then P_a has volume (independently of a)

$$|P_a| = 4 \int\limits_0^{2a} f_a(x) \, dx = 4 \int\limits_0^{2a} -\frac{8}{a^2}x + \frac{16}{a} \, dx = 64$$

and second central moment (depending on a)

$$\begin{aligned} \mu_2(P_a) &= \frac{1}{|P_a|} \int\limits_{P_a} |x|^2 \, dx = \frac{4}{64} \int\limits_0^{2a} \int\limits_0^{-\frac{8}{a^2}x_2 + \frac{16}{a}} x_1^2 + x_2^2 \, dx_1 \, dx_2 \\ &= \frac{2}{3} \frac{(a^4 + 64)}{a^2}. \end{aligned}$$

We next determine the value for $a > 0$ such that $\mu_2(R_a) = \mu_2(P_a)$, i.e.,

$$\frac{16}{3} \frac{(a^4+1)}{a^2} = \frac{2}{3} \frac{(a^4+64)}{a^2} \iff a = \sqrt[4]{8}.$$

For abbreviation we set $R := R_{\sqrt[4]{8}}$ and $P := P_{\sqrt[4]{8}}$. So we have

$$|R| = |P| = 64 \qquad \text{and} \qquad \mu_2(R) = \mu_2(P) = 768\sqrt{2}.$$

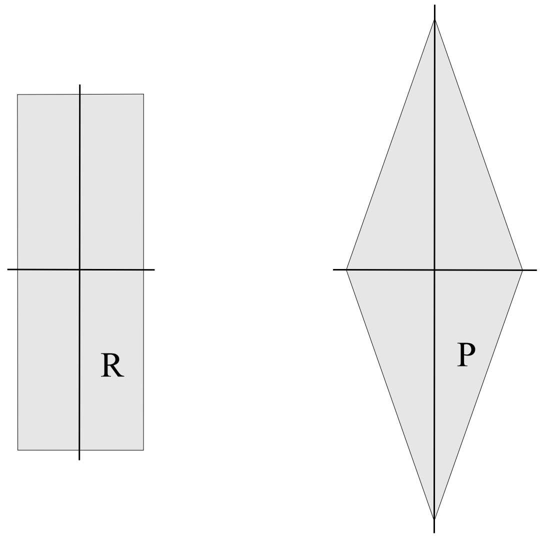

Figure 3.4: R and P.

The fourth central moments are given by

$$\begin{aligned}\mu_4(R) &= \frac{1}{64}\int\limits_R |x|^4\,dx = \frac{4}{64}\int\limits_0^{4a}\int\limits_0^{\frac{4}{a}} x_1^4 + 2\,x_1^2\,x_2^2 + x_2^4\,dx_1\,dx_2 \\ &= \frac{256}{45}\frac{(9a^8+10a^4+9)}{a^4}\Big|_{a=\sqrt[4]{8}} = \frac{4256}{9} \approx 472,89\end{aligned}$$

and

$$\begin{aligned}\mu_4(P) &= \frac{1}{64}\int\limits_P |x|^4\,dx = \frac{4}{64}\int\limits_0^{2a}\int\limits_0^{-\frac{8}{a^2}x_2+\frac{16}{a}} x_1^4 + 2\,x_1^2\,x_2^2 + x_2^4\,dx_1\,dx_2 \\ &= \frac{16}{45}\frac{(3a^8+64a^4+12288)}{a^4}\Big|_{a=\sqrt[4]{8}} = \frac{25984}{45} \approx 577,42,\end{aligned}$$

i.e., we have

$$\mu_4(R) < \mu_4(P).$$

We now show that the Hilbert-Schmidt norms of Θ^R and Θ^P are equal. For Θ^R it is given by

$$\begin{aligned}\|\Theta^R\|_{HS}^2 &= \sum_{i,j=1}^{2}(\Theta_{ij}^R)^2 = \sum_{i,j=1}^{2}\Big(\int\limits_R x_i x_j\,dx\Big)^2 \\ &= \Big(\int\limits_R x_1^2\,dx\Big)^2 + \Big(\int\limits_R x_2^2\,dx\Big)^2 + 2\underbrace{\Big(\int\limits_R x_1 x_2\,dx\Big)^2}_{=0},\end{aligned}$$

where the last summand vanishes by the symmetries of R with respect to the x_1- and x_2-axis (and clearly the last summand also vanishes for Θ^P). So we have

$$\begin{aligned} \|\Theta^R\|_{HS}^2 &= \Big(\int_R x_1^2\,dx\Big)^2 + \Big(\int_R x_2^2\,dx\Big)^2 \\ &= \Big(4\int_0^{4a}\int_0^{\frac{4}{a}} x_1^2\,dx_1\,dx_2\Big)^2 + \Big(4\int_0^{4a}\int_0^{\frac{4}{a}} x_2^2\,dx_1\,dx_2\Big)^2 \\ &= 2\Big(\frac{256}{3}\Big)^2 + 2\Big(\frac{2048}{3}\Big)^2 \end{aligned}$$

and

$$\begin{aligned} \|\Theta^P\|_{HS}^2 &= \Big(4\int_0^{2a}\int_0^{-\frac{8}{a^2}x_2+\frac{16}{a}} x_1^2\,dx_1\,dx_2\Big)^2 + \Big(4\int_0^{2a}\int_0^{-\frac{8}{a^2}x_2+\frac{16}{a}} x_2^2\,dx_1\,dx_2\Big)^2 \\ &= 2\Big(\frac{256}{3}\Big)^2 + 2\Big(\frac{2048}{3}\Big)^2. \end{aligned}$$

Finally, since $|R| = |P|$, $\mu_2(R) = \mu_2(P)$, $\mu_4(R) < \mu_4(P)$ and $\|\Theta^R\|_{HS} = \|\Theta^P\|_{HS}$ it follows by Theorem 52 that there exists a critical time $t_2 \in (0,\infty)$ such that

$$\|T(t)\mathbb{1}_R\|_{L^2} < \|T(t)\mathbb{1}_P\|_{L^2}, \qquad t > t_2.$$

3.4 Final considerations

One could ask the question: How much geometry of D is determined by the flow $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$?

The following is an interesting consequence of our main results in Chapter 2 and 3 and gives a partial answer.

Theorem 55. *Let $A, D \subset \mathbb{R}^n$ be two Caccioppoli sets and $(t_n)_{n\in\mathbb{N}}$ a sequence with accumulation point in $(0,\infty)$. If*

$$\|T(t_n)\mathbb{1}_A\|_{L^2} = \|T(t_n)\mathbb{1}_D\|_{L^2} \qquad \textit{for every } n \in \mathbb{N},$$

then A and D have

i) the same volume $|A| = |D|$,
ii) the same perimeter $P(A) = P(D)$ and
iii) the same distance integrals

$$\int_A\int_A |x-y|^{2k}\,dx\,dy = \int_D\int_D |x-y|^{2k}\,dx\,dy \qquad \textit{for every } k \in \mathbb{N}.$$

Proof: By the analyticity of $t \mapsto \|T(t)\mathbb{1}_A\|_{L^2}$ and $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$, see Chapter 1, Remark 2, the condition

$$\|T(t_n)\mathbb{1}_A\|_{L^2} \;=\; \|T(t_n)\mathbb{1}_D\|_{L^2} \qquad \text{for every } n \in \mathbb{N},$$

implies that the two maps coincide for every $t \in (0, \infty)$. By continuity they also coincide for $t = 0$. So we have

$$\|T(t)\mathbb{1}_A\|_{L^2} \;=\; \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \geq 0. \tag{3.23}$$

This yields $|A| = |D|$ and $P(A) = P(D)$ since

$$\|T(0)\mathbb{1}_D\|_{L^2}^2 = |D|$$

and

$$\begin{aligned}
\lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \Big(|D| - \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2 \Big) &= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \Big(|D| - \langle T(t)\mathbb{1}_D, \mathbb{1}_D \rangle \Big) \\
&= \lim_{t\to 0} \frac{\sqrt{\pi}}{\sqrt{t}} \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c} \rangle \\
&= P(D).
\end{aligned}$$

Furthermore, all the integrals

$$\int_A \int_A |x-y|^{2k}\, dx\, dy \;=\; \int_D \int_D |x-y|^{2k}\, dx\, dy \qquad \text{for every } k \in \mathbb{N}$$

must coincide since an inequality

$$\int_A \int_A |x-y|^{2k_0}\, dx\, dy < \int_D \int_D |x-y|^{2k_0}\, dx\, dy \qquad \text{for some } k_0 \in \mathbb{N}$$

would imply by Proposition 43 that (3.23) could not hold for all $t \geq 0$. □

Final Conjecture 56. It seems to be an open question whether the above properties i)-iii) imply that A und D have additional common properties or maybe that they already have to be congruent.

If this would be true, we could - up to a rigid motion - characterise a compact set D by the induced evolution $t \mapsto \|T(t)\mathbb{1}_D\|_{L^2}$, and even by its values on a sequence $(t_n)_{n\in\mathbb{N}}$ with accumulation point in $(0, \infty)$.

This is reminiscent of the famous question of M. Kac [Kac66]: "Can one hear the shape of a drum?", i.e., does the sequence $(\lambda_n)_{n\in\mathbb{N}}$ of Dirichlet eigenvalues of D determine the geometry of D. There, as shown by a counterexample of C. Gordon, D.L. Webb, S. Wolpert [GWW92] the answer is, in general, negative.

So we dare to close with the question: "With a perfect measuring instrument for heat, can one deduce the shape of a coffee cup?"

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Zusammenfassung in deutscher Sprache

Wir betrachten eine gleichmäßige Wärmeverteilung in einer kompakten Menge D des $\mathbb{R}^n$, die durch die charakteristische Funktion $\mathbb{1}_D$ of D repräsentiert wird. Die Wärmeleitungshalbgruppe $(T(t))_{t\geq 0}$ auf $L^2(\mathbb{R}^n)$ liefert dann, angewandt auf $\mathbb{1}_D$, die eindeutige Lösung $u(x,t) = T(t)\mathbb{1}_D(x)$ der Wärmeleitungsgleichung

$$\text{(WLG)} \qquad \begin{cases} \frac{d}{dt}u(x,t) = \Delta u(x,t), & x \in \mathbb{R}^n, t \geq 0, \\ u(x,0) = \mathbb{1}_D(x) \end{cases}$$

auf $\mathbb{R}^n$ für alle Zeiten $t \geq 0$ mit Anfangswert $\mathbb{1}_D$.
Dieser Wärmefluss induziert insbesondere eine Evolution der entsprechenden L^2-Normen

$$t \quad \mapsto \quad \|T(t)\mathbb{1}_D\|_{L^2}, \qquad t \geq 0. \tag{1}$$

Wenn wir die Notation

$$\langle f, g\rangle := \int_{\mathbb{R}^n} f(x) \cdot g(x)\, dx$$

sowohl für das innere Produkt auf $L^2(\mathbb{R}^n)$ als auch für das duale Paar $\langle L^1(\mathbb{R}^n), L^\infty(\mathbb{R}^n)\rangle$ verwenden, dann bekommen wir mit der Halbgruppeneigenschaft

$$T(t+s)\mathbb{1}_D = T(t)T(s)\mathbb{1}_D, \qquad s,t \geq 0$$

und der Selbstadjungiertheit der Operatoren $T(t)$ die folgende alternative Form der Evolution (1):

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = \langle T(\tfrac{t}{2})\mathbb{1}_D, T(\tfrac{t}{2})\mathbb{1}_D\rangle = \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2, \qquad t \geq 0. \tag{2}$$

Da zudem im $\mathbb{R}^n$ unter Diffusion keine Wärme verloren geht, liefert dies auch

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = |D| - \langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = |D| - \|T(\tfrac{t}{2})\mathbb{1}_D\|_{L^2}^2, \quad t \geq 0. \tag{3}$$

Mit der Integralschreibweise

$$\langle T(t)\mathbb{1}_D, \mathbb{1}_D\rangle = \int_D T(t)\mathbb{1}_D(x)\, dx \quad \text{und} \quad \langle T(t)\mathbb{1}_D, \mathbb{1}_{D^c}\rangle = \int_{D^c} T(t)\mathbb{1}_D(x)\, dx$$

wird deutlich, dass (2) genau die Wärmemenge beschreibt, die zur Zeit t noch in D ist, während (3) angibt, was bereits ins Komplement D^c geflossen ist. In diesem Sinne spiegelt die Entwicklung der L^2-Normen (1) wider, wie gut die Menge D Wärme in sich hält.

Im *ersten Kapitel* geben wir eine kurze Zusammenfassung der analytischen und geometrischen Konzepte, die im weiteren benutzt werden. Wir führen die Wärmeleitungshalbgruppe auf $\mathbb{R}^n$ und ihre wichtigsten Eigenschaften ein. Wir gehen auf das Konzept der Symmetrisierung im $\mathbb{R}^n$ und die Riesz-Sobolev-Ungleichung ein und zeigen interessante, aber weitgehend unbekannte Beziehungen zwischen der Wärmeleitungshalbgruppe und Symmetrisierungs-Ungleichungen. Weiter stellen wir kurz den nötigen Hintergrund zum Perimeter, relevante geometrische Maßtheorie und grundlegende Begriffe der Geometrie glatter Hyperflächen im $\mathbb{R}^n$ vor.

Im *zweiten Kapitel* konzentrieren wir uns auf das Kurzzeitverhalten des Flusses $t \mapsto T(t)\mathbb{1}_D$. Wir beginnen mit einer genauen Untersuchung der Evolution der Niveauflächen von $T(t)\mathbb{1}_D$ und bestimmen das asymptotische Verhalten dieser Evolution: Wir zeigen, dass für kurze Zeiten die Bewegung der Niveauflächen eine asymptotische Entwicklung in Potenzen von $t^{1/2}$ besitzt. Wir bestimmen die Koeffizienten bis zur Ordnung t^2 in Termen geometrischer Invarianten des Randes ∂D und geben eine allgemeine Formel für die Koeffizienten höherer Ordnung an.
Wir zeigen dann, dass das Kurzzeitverhalten des Flusses (1)-(3) für eine beliebige Caccioppoli-Menge D durch den Perimeter von D kontrolliert ist.
Als Folgerung erhalten wir einen Vergleichssatz, der sagt, dass für zwei beliebige kompakte volumengleiche Mengen $A, D \subset \mathbb{R}^n$ diejenige mit dem kleineren Perimeter für kurze Zeiten Wärme besser hält als die andere.

Im *dritten Kapitel* konzentrieren wir uns auf Langzeitphänomene des Flusses (1)-(3). Vor allem betrachten wir das Analogon der Frage, die wir am Ende von Kapitel 2 behandelt haben: Gegeben seien zwei kompakte volumengleiche Mengen $A, D \subset \mathbb{R}^n$. Welche hält für lange Zeiten Wärme besser?
Wir beweisen wiederum einen Vergleichssatz, der sagt, dass dieses für diejenige Menge gilt, die kleineres zweites Zentralmoment hat. Darüberhinaus geben wir Kriterien für die vierten Zentralmomente und die Trägheitstensoren von A and D an für den Fall, dass die zweiten Zentralmomente gleich sind.

Wir schließen die Arbeit mit Überlegungen zu der Frage, wie viel Geometrie von D bereits bestimmt ist, wenn wir den Fluss (1)-(3) auf einem (eventuell kleinen) Zeitintervall kennen.

Lebenslauf

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