Shedding new light on Gaussian harmonic analysis

Teuwen, Jonas

DOI
10.4233/uuid:bcfb2d09-5828-4ad8-bfe6-e6cfe3b83c3f

Publication date
2016

Document Version
Final published version

Citation (APA)
Teuwen, J. (2016). *Shedding new light on Gaussian harmonic analysis*. [Dissertation (TU Delft), Delft University of Technology]. https://doi.org/10.4233/uuid:bcfb2d09-5828-4ad8-bfe6-e6cfe3b83c3f

SHEDDING NEW LIGHT ON GAUSSIAN HARMONIC ANALYSIS

Jonas Teuwen

Shedding new light on Gaussian harmonic analysis

Shedding new light on Gaussian harmonic analysis

Proefschrift

ter verkrijging van de graad van doctor
aan de Technische Universiteit Delft,
op gezag van de Rector Magnificus prof. ir. K.C.A.M. Luyben,
voorzitter van het College voor Promoties,
in het openbaar te verdedigen op dinsdag 29 maart 2016 om 12:30 uur

door

Jonas Jan Bart Teuwen

Wiskundig ingenieur,
geboren te Harelbeke, België.

Dit proefschrift is goedgekeurd door de

promotor 1: Prof. dr. J.M.A.M. van Neerven
promotor 2: Prof. dr. H.P. Urbach

Samenstelling promotiecommissie:

Rector Magnificus,	voorzitter
Prof. dr. J.M.A.M. van Neerven,	Technische Universiteit Delft
Prof. dr. H.P. Urbach,	Technische Universiteit Delft
Onafhankelijke leden:	
Prof. dr. B. de Pagter,	Technische Universiteit Delft
Dr. S.F. Pereira,	Technische Universiteit Delft
Dr. P. Portal,	Australian National University
Prof. dr. F.H.J. Redig,	Technische Universiteit Delft
Prof. dr. F. Vallentin,	Universität zu Köln
Overige leden:	
Prof. dr. ir. G. Jongbloed,	Technische Universiteit Delft

Het onderzoek beschreven in dit proefschrift is mede gefinancierd door de Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), door de NWO-VICI onder projectnummer 639.033.604.

Netherlands Organisation for Scientific Research

Keywords: Ornstein-Uhlenbeck semigroup, Mehler kernel, Gaussian maximal function, admissible cones, Mehler kernel bounds, off-diagonal estimates, infinite-dimensional optimization

Cover design: Fay van Leeuwen and Lucas Rozenboom

An electronic version of this dissertation is available at `http://repository.tudelft.nl/`.

This dissertation is so dry not even a cactus could grow on it.

Contents

I.

Mathematics

1.
Introduction

1.1. Introduction

This chapter contains a summary of many well-known results related to the Hermite polynomials and the Ornstein-Uhlenbeck semigroup. It is intented to sketch the general context in which the results of Chapters 2-4 should be seen.

In the first part we sketch the general setting and give the relationship between the Gaussian measure, from which the field “Gaussian Harmonic Analysis” borrows its name, and the *Ornstein-Uhlenbeck operator* which is our main object of study. Furthermore, several equivalent definitions of the Hermite polynomials are given. Some basic results such as the binomial identity for the Hermite polynomials will show how these polynomials can be treated in a quite elementary fashion. The main result which we will prove in this part is that the Hermite polynomials are dense, and form an orthonormal basis for the L^2 space associated with the Gaussian measure. We will give an elementary proof of this fact.

The second part concerns the *Mehler kernel*, which is the associated integral kernel to these operators.

As an addition, in the last part we give a proof based on an idea by [1] of the celebrated *uncertainty principle* from Fourier analysis using the Hermite polynomials.

1.1.1. The notation

In his dissertation, we will denote the number fields by a bold face capital letter. For instance, **R** denotes the real line. Common spaces such as L^2 against a certain measure μ will often be denoted by L^2_μ for simplicity as opposed to $L^2(\mu)$ or $L^2(\mathbf{R}^d, \mu)$ when more detail is required. In a similar spirit we will denote the Lebesgue measure by $\mathrm{d}\lambda$ whenever we suppress the argument in an integral, otherwise $\mathrm{d}x$ and the like will be used. As is usual, the Laplacian on $\mathbf{R}^d$ is denoted by Δ. That is

$$\Delta := \nabla \cdot \nabla = \nabla^2 = \sum_{i=1}^{d} \partial_i^2.$$

1.2. Hermite? Gaussian? On a measure

There are many equivalent definitions for the Hermite polynomials. The way one in harmonic analysis and partial differential equations usually introduces the Hermite polynomials is by first introducing the *Gaussian measure*.

1.2.1. Gaussian and Hilbertian

The *Gaussian* on $\mathbf{R}^d$ is commonly used to refer to the function γ defined by

$$\gamma(x) := \frac{\mathrm{e}^{-|x|^2}}{\pi^{\frac{d}{2}}}. \tag{1.1}$$

where $|x| = x_1^2 + \cdots + x_d^2$. Associated to the Gaussian we can define the *Gaussian measure*,

$$\mathrm{d}\gamma(x) = \gamma(\mathrm{d}x) = \mathrm{e}^{-|x|^2} \frac{\mathrm{d}x}{\pi^{\frac{d}{2}}}. \tag{1.2}$$

There are some other choices for the Gaussian γ as well, related to their probabilistic interpretation as the density for the *normal distribution*. In probability theory one would have for the standard normal random variable[1] $X \sim N(0, I)$, with mean $\mu = 0$ and variance $\sigma^2 = 1$. Then X would have the density of the *standard Gaussian* $\tilde{\gamma}$ which is given by

$$\tilde{\gamma}(x) := \frac{\mathrm{e}^{-|x|^2/2}}{\sqrt{2\pi}}.$$

It would be perfectly feasible, and would yield equivalent results to use the standard Gaussian in what follows. But in recent literature, e.g. [8] the Gaussian as in (1.1) is used and we will follow this convention.

In general, we will work in the d-dimensional space $\mathbf{R}^d$, except when we can reduce to the one-dimensional case (as is done in Chapter 3). Using (1.1), the *Gaussian Hilbert space* $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ is the L^2-space on $\mathbf{R}^d$ with the Gaussian measure $\mathrm{d}\gamma$ and the inner product defined by

$$\langle u, v\rangle_{L^2(\mathbf{R}^d,\mathrm{d}\gamma)} := \langle u, v\rangle = \int_{\mathbf{R}^d} u\bar{v}\,\mathrm{d}\gamma.$$

The norm on $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ is the *induced norm* by the inner product. So, $\|\cdot\|_{L^2(\mathbf{R}^d,\mathrm{d}\gamma)}$ is

$$\|u\|_{L^2(\mathbf{R}^d,\mathrm{d}\gamma)} := \sqrt{\langle u, u\rangle} = \left(\int_{\mathbf{R}^d} |u|^2\,\mathrm{d}\gamma\right)^{1/2}. \tag{1.3}$$

On the usual L^2-space with the Lebesgue measure the Laplacian Δ is symmetric. This means that

$$\int_{\mathbf{R}^d} u\Delta v\,\mathrm{d}\lambda = \int_{\mathbf{R}^d} v\Delta u\,\mathrm{d}\lambda, \quad u, v \in C_c^2(\mathbf{R}^d).$$

[1] I is the $d \times d$ identity matrix.

One has to be a bit careful here, as Δ is an *unbounded operator*, the symmetric property of an operator not only depends on the action of the operator itself, but additionally it depends on the *domain*[2]. Note that Δ is not symmetric on $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$. Computing we get that

$$\begin{aligned}\int_{\mathbf{R}^d} u\partial_i v \,\mathrm{d}\gamma &= \frac{1}{\sqrt{\pi}}\int_{\mathbf{R}^d} u(x)\mathrm{e}^{-|x|^2}\partial_i v(x)\,\mathrm{d}x \\ &= -\int_{\mathbf{R}^d} \partial_i uv \,\mathrm{d}\gamma + \int_{\mathbf{R}^d} 2x_i uv \,\mathrm{d}\gamma.\end{aligned}$$

From this we can conclude that the adjoint ∂_i^* of ∂_i in $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ is given by

$$\partial_i^* = -\partial_i + 2x_i. \tag{1.4}$$

Taking this into account, we define the symmetric operator on $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ analoguous to the Laplacian to be

$$L := -\frac{1}{2}\sum_{i=1}^{d} \partial_i^* \partial_i. \tag{1.5}$$

The factor here $\frac{1}{2}$ is merely for convenience, as it gives rise to nicer expressions. The operator L is the so-called *Ornstein-Uhlenbeck* operator. Note that we can write the Ornstein-Uhlenbeck operator (1.5) using (1.4) in Euclidean coordinates as

$$L = \frac{1}{2}\Delta - \langle x, \nabla\rangle. \tag{1.6}$$

In the next sections we will introduce the Hermite polynomials and show that these form an orthogonal basis for $L^2(\mathbf{R}, \mathrm{d}\gamma)$, and more importantly, that these are the eigenfunctions of the Ornstein-Uhlenbeck operator L.

[2] Some good references on these aspects of unbounded operators are [2, 9].

1.2.2. Hermite and his polynomials

The Hermite polynomials form a certain subclass of the so-called *orthogonal polynomials* which are one of the main objects of study in the field of *special functions*. For Hermite polynomials the Gaussian integral plays an important role,

$$\int_{\mathbf{R}} e^{-x^2}\,dx = \sqrt{\pi}. \tag{1.7}$$

Comparing this integral with the Gaussian measure (1.2) for $d = 1$, we can see that $d\gamma$ is a *probability measure*, i.e., the whole space has measure one. Moreover, the Gaussian γ has many additional nice properties. For instance, γ is up to a multiplicative constant a fixed point for the Fourier transform[3]. In fact there holds that

$$e^{-x^2} = \frac{1}{\sqrt{\pi}} \int_{\mathbf{R}} e^{-2ix\xi} e^{-\xi^2}\,d\xi. \tag{1.8}$$

To see this, set $v(x) = e^{-x^2}$ and note that

$$\partial_x v(x) = -2xv(x). \tag{1.9}$$

We will proceed by computing the Fourier transform

$$\mathscr{F}(u)(x) := \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} u(\xi) e^{-ix\xi}\,d\xi, \quad u \in L^1(\mathbf{R}), \tag{1.10}$$

of the left- and right-hand side of (1.9). Recall that

$$\mathscr{F}(u')(x) = ix\mathscr{F}(u)(x),$$
$$\mathscr{F}(u)(x)' = i\mathscr{F}(\xi \mapsto \xi u(\xi))(x).$$

[3] Up to a multiplicative constant which depends on the chosen normalization of the Fourier transform.

Applying these identities to (1.9) we get

$$ix\mathscr{F}(v)(x) = -2i\partial_x \mathscr{F}(v)(x).$$

Rearranging and integrating we get

$$-\frac{1}{4}x^2 = \int_0^x \frac{\partial_\xi \mathscr{F}(v)(\xi)}{\mathscr{F}(v)(\xi)}\,\mathrm{d}\xi = \log \mathscr{F}(v)(x) - \log \mathscr{F}(v)(0).$$

Taking exponentials, and noting that by (1.7) we have $\mathscr{F}(v)(0) = \frac{1}{\sqrt{2}}$ so we get

$$\mathrm{e}^{-\frac{1}{4}x^2} = \frac{1}{\pi}\int_{\mathbf{R}} \mathrm{e}^{-ix\xi}\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi.$$

Substituting $x \to 2x$ yields (1.8), completing the proof.

We now *define* the Hermite polynomials through their *Rodrigues' formula* which is given by,

$$H_n(x) := (-1)^n \mathrm{e}^{x^2}\partial_x^n \mathrm{e}^{-x^2}. \tag{1.11}$$

From the definition (1.11) we can also verify by induction that H_n is a polynomial of degree n, hence justifying their nomenclature. Using Theorem 1.2 from Section 1.5 we obtain for all x that differentiation under the integral sign in (1.8) is allowed. Doing this, we get

$$\partial_x^n \mathrm{e}^{-x^2} = \frac{(2i)^n}{\sqrt{\pi}}\int_{\mathbf{R}} \mathrm{e}^{2ix\xi}\xi^n \mathrm{e}^{-\xi^2}\,\mathrm{d}\xi.$$

Together with the Rodrigues formula (1.11) we immediately get an equivalent integral definition for the Hermite polynomials.

$$H_n(x) = \frac{(-2i)^n \mathrm{e}^{x^2}}{\sqrt{\pi}}\int_{\mathbf{R}} \xi^n \mathrm{e}^{2ix\xi}\mathrm{e}^{-\xi^2}\,\mathrm{d}\xi. \tag{1.12}$$

Another property which will give us some fruitful results is their orthogonality. Using δ_{mn} to denote the *Kronecker delta*[4], we have

$$\langle H_n, H_m \rangle_\gamma = \int_{\mathbf{R}} H_n(x) H_m(x) \gamma(\mathrm{d}x) = 2^n n! \delta_{mn}. \tag{1.13}$$

This is an important property and requires proof. We start with the case $m > n$, while the case $m < n$ is the same and the case $m = n$ will be handled later on. We can write the integral in (1.13) with H_n as in the Rodrigues formula (1.11). That is,

$$\langle H_n, H_m \rangle_\gamma \overset{(1.11)}{=} \frac{(-1)^m}{\sqrt{\pi}} \int_{\mathbf{R}} H_n(x) \partial_x^m \mathrm{e}^{-x^2} \,\mathrm{d}x.$$

Noting that $\partial_x^m \mathrm{e}^{-x^2} = p_m(x)\mathrm{e}^{-x^2}$ where $p_m(x)$ is a polynomial in x of m^{th} degree we get by induction for $m > n$,

$$\begin{aligned}
\langle H_n, H_m \rangle_\gamma &= \frac{(-1)^m}{\sqrt{\pi}} \left\{ \Big[H_n(x) p_{m-1}(x) \mathrm{e}^{-x^2} \Big]_{-\infty}^{\infty} - \int_{\mathbf{R}} H_n(x)' \partial_x^{m-1} \mathrm{e}^{-x^2} \,\mathrm{d}x \right\} \\
&= \dots \\
&= \frac{1}{\sqrt{\pi}} \int_{\mathbf{R}} (\partial_x^m H_n(x)) \mathrm{e}^{-x^2} \,\mathrm{d}x = 0,
\end{aligned}$$

where all the boundary terms vanish as e^{-x^2} decays faster than any polynomial and $\partial_x^m H_n(x) = 0$ as $m > n$. Switching the rôles of m and n shows $\langle H_n, H_m \rangle_\gamma = 0$ whenever $m \neq n$.

The case $n = m$ is only slightly harder, but it requires some careful bookkeeping. To be able to handle this case, we do need to know what the effect of differentiation is on the Hermite polynomials. To investigate such properties for orthogonal polynomials, the *generating function* often comes

[4] Recall that δ_{mn} is the Kronecker delta which is 1 whenever $m = n$ or 0 otherwise.

in handy. The generating function h for the Hermite polynomials $(H_n)_n$ is defined as

$$h(x,t) := \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n.$$

We have already cooked up all ingredients needed to evaluate this series. Using (1.12) we have

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n &\overset{(1.12)}{=} \int_{\mathbf{R}} \sum_{n=0}^{\infty} \frac{(-2it)^n}{n!} \xi^n \mathrm{e}^{(x+i\xi)^2} \frac{\mathrm{d}\xi}{\sqrt{\pi}} \\ &= \int_{\mathbf{R}} \mathrm{e}^{-2it\xi} \mathrm{e}^{(x+i\xi)^2} \frac{\mathrm{d}\xi}{\sqrt{\pi}}.\end{aligned}$$

The last integral is one we have seen already. After a change of variables and using (1.8) we see that the generating function h is given by

$$h(x,t) = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n = \mathrm{e}^{-(x-t)^2+x^2} = \mathrm{e}^{2xt-t^2}. \tag{1.14}$$

The case $n = m$ of (1.13) corresponds to the $L^2(\mathbf{R}, \mathrm{d}\gamma)$ norm (1.3) squared, and for us to be able to swifty deduce the $L^2(\mathbf{R}, \mathrm{d}\gamma)$ norm of the Hermite polynomials, we first need some other results which are interesting in their own right as well. To refine the proof of (1.13) for the case $n = m$, we would like to know more about $\partial_x^n H_n(x)$. For this, we use the generating function h from (1.14). Note that the derivative of h with respect to t gives

$$\partial_t \sum_{n=0}^{\infty} H_n(x) \frac{t^n}{n!} = \sum_{n=0}^{\infty} H_{n+1}(x) \frac{t^n}{n!}.$$

Next, we use a nice property of the generating function, namely

$$\partial_t h(x,t) = (2x - \partial_x) h(x,t).$$

Putting these things together gives

$$\sum_{n=0}^{\infty} H_{n+1}(x)\frac{t^n}{n!} = \sum_{n=0}^{\infty}[2xH_n(x) - H_n'(x)]\frac{t^n}{n!}.$$

Equating coeffficients, we can deduce the *recursion relation*

$$H_n'(x) = H_{n+1}(x) - 2xH_n(x). \tag{1.15}$$

There is also another way to compute the derivative of H_n. Taking the derivative of the Rodrigues formula (1.11) for H_n. We get

$$H_n'(x) = 2x(-1)^n e^{x^2}\partial_x^n e^{-x^2} + 2x(-1)^n e^{x^2}\partial_x^{n+1} e^{-x^2}.$$

This gives us another way to derive (1.15). Differentiating the series representation of the generating function k times with respect to t gives

$$\partial_t^n \sum_{k=0}^{\infty} \frac{H_k(x)}{k!} t^k = \sum_{k=n}^{\infty} \frac{H_k(x)}{(k-n)!} t^{k-n}.$$

Which allows us to conclude that the n^{th} Hermite polynomial H_n is equal to

$$H_n(x) = \partial_t^n h(x,t)\Big|_{t=0} = (\partial_t^n e^{2xt-t^2})\Big|_{t=0}. \tag{1.16}$$

This is interesting, as we can differentiate this expression easily with respect to x as well. That is

$$H_n'(x) = (\partial_t^n 2t e^{2xt-t^2})\Big|_{t=0}.$$

Applying the product rule to the term on the right-hand side gives

$$\begin{aligned}\partial_t^n(2te^{2xt-t^2}) &= \sum_{k=0}^{n}\binom{n}{k}(\partial_t^{n-k}e^{2xt-t^2})(\partial_t^k 2t)\\ &= 2t\partial_t^n e^{2xt-t^2} + 2n\partial_t^{n-1}e^{2xt-t^2}.\end{aligned}$$

Hence, for $t = 0$, there is only one non-zero term in the expansion. Thus we get

$$H_n'(x) = (\partial_t^n 2t\mathrm{e}^{2xt-t^2})\Big|_{t=0} = (2n\partial_t^{n-1}\mathrm{e}^{2xt-t^2})\Big|_{t=0}.$$

Matching this result with (1.16), we conclude that

$$H_n'(x) = 2nH_{n-1}(x). \tag{1.17}$$

Combining with (1.15) we obtain

$$H_{n+1}(x) - 2xH_n(x) = 2nH_{n-1}(x). \tag{1.18}$$

This time everything is in place to compute the $L^2(\mathbf{R}, \mathrm{d}\gamma)$ norm of the Hermite polynomials. We proceed as before. By (1.11) we get, using integration by parts

$$\begin{aligned}\int_{\mathbf{R}} H_n^2 \,\mathrm{d}\gamma &= (-1)^n \int_{\mathbf{R}} H_n(x)\partial_x^n \,\mathrm{e}^{-x^2} \frac{\mathrm{d}x}{\sqrt{\pi}} \\ &= (-1)^{n-1} \int_{\mathbf{R}} H_n'(x)\partial_x^{n-1} \,\mathrm{e}^{-x^2} \frac{\mathrm{d}x}{\sqrt{\pi}}.\end{aligned}$$

We can now apply (1.17) to the last line, and obtain using integration by parts that

$$\int_{\mathbf{R}} H_n^2 \,\mathrm{d}\gamma = 2^n n! \int_{\mathbf{R}} H_0(x)\,\mathrm{e}^{-x^2} \frac{\mathrm{d}x}{\sqrt{\pi}}.$$

In conclusion we get after noting that $H_0 = 1$ together with the Gaussian integral (1.7) that the $L^2(\mathbf{R}, \mathrm{d}\gamma)$ norm of H_n is

$$\|H_n\|^2_{L^2(\mathbf{R},\mathrm{d}\gamma)} = \langle H_n, H_n\rangle_{L^2(\mathbf{R},\mathrm{d}\gamma)} = \int_{\mathbf{R}} H_n^2 \,\mathrm{d}\gamma = 2^n n!.$$

In particular this also proves the case $n = m$ for the orthogonality condition (1.13). This concludes the proof that the Hermite polynomials form an orthogonal set of $L^2(\mathbf{R}, d\gamma)$. We now set h_n to be the *normalized Hermite polynomial* H_n, that is,

$$h_n = \frac{H_n}{\sqrt{2^n n!}} \quad \text{such that} \quad \langle h_n, h_m \rangle = \delta_{nm}. \tag{1.19}$$

In the next section we will show that not only the set $(H_n)_n$ is orthogonal, but that it is additionally *complete*. This will allow us to express any function in $L^2(\mathbf{R}, d\gamma)$ in terms of the Hermite polynomials.

1.2.3. The Hermite basis is complete

One of the most important properties from a functional analytic point of view is that the Hermite polynomials $(H_n)_n$ form a *complete set*, i.e., a *basis*. The *completeness* of (H_n) can be defined using the following two equivalent properties:

1. $\operatorname{span}\{H_n : n \in \mathbf{N}\}$ is *dense* in $L^2(\mathbf{R}, d\gamma)$;

2. For any u in $L^2(\mathbf{R}, d\gamma)$ we can find unique scalars (a_n) such that u can be expressed in the form:

$$u = \sum_{n=0}^{\infty} a_n H_n,$$

   where the convergence is in $L^2(\mathbf{R}, d\gamma)$.

We proceed with proving condition 1 for the Hermite polynomials. Note that we could rephrase the first condition using the orthogonal decomposition of $L^2(\mathbf{R}, d\gamma)$ in terms of the linear span of all Hermite polynomials $\mathscr{H}$ and its orthogonal complement. That is, we set

$$\mathscr{H} := \operatorname{span}\{H_n : n \in \mathbf{N}\}.$$

In order for $\mathscr{H}$ to be a dense set, the closed linear span

$$\overline{\text{span}}\{H_n : n \in \mathbf{N}\},$$

should be dense in $L^2(\mathbf{R}, \mathrm{d}\gamma)$, where the bar denotes the closure. Now we decompose $L^2(\mathbf{R}, \mathrm{d}\gamma)$ into the direct sum of $\mathscr{H}$ and its orthogonal complement. That is

$$L^2(\mathbf{R}, \mathrm{d}\gamma) = \mathscr{H} \oplus \mathscr{H}^{\perp}.$$

If u is in $\mathscr{H}^{\perp}$ we have

$$\int_{\mathbf{R}} H_n(x)u(x)\,\mathrm{e}^{-x^2}\frac{\mathrm{d}x}{\sqrt{\pi}} = 0, \tag{1.20}$$

for all n in $\mathbf{N}$. Our goal is to prove that the integrals in (1.20) vanish for all $n \in \mathbf{N}$ if and only if $u = 0$ is almost everywhere. This will show that (H_n) has dense span in $L^2(\mathbf{R}, \mathrm{d}\gamma)$.

We will actually show that the span of the set $(x \mapsto x^n)_n$ of functions is dense in $L^2(\mathbf{R}, \mathrm{d}\gamma)$. As we can express any such function as a finite linear combinations of Hermite polynomials, this will prove the result. So, let $u \perp \text{span}\{x^n : n \in \mathbf{N}\}$. To prove the density we introduce the function U given by

$$U(z) := \frac{1}{\sqrt{2\pi}}\int_{\mathbf{R}} u(x)\mathrm{e}^{zx}\mathrm{e}^{-x^2}\,\mathrm{d}x, \quad z \in \mathbf{C}.$$

The first thing we can note is that U defines an *entire function* of the complex variable z, which means that U is everywhere holomorphic on $\mathbf{C}$. Next, we express e^{zx} int its Taylor series, by Fubini's theorem we can then interchange sum and integral to obtain

$$U(z) = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\mathbf{R}} u(x) x^n \mathrm{e}^{-x^2} \,\mathrm{d}x.$$

Per assumption that u is orthogonal to each polynomial we note that $U(z) = 0$ for each z in $\mathbf{C}$. This allows us to set $z = -i\xi$ and conclude that $U(-i\xi)$ vanishes too. Note that

$$U(-i\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} u(x) \mathrm{e}^{-ix\xi} \mathrm{e}^{-x^2} \,\mathrm{d}x = \mathscr{F}(x \mapsto \mathrm{e}^{-x^2} u(x))(\xi).$$

That is, $U(-i\xi)$ is the *Fourier transform* (1.10) of $x \mapsto \mathrm{e}^{-x^2} u(x)$, and that the Fourier transform of this function vanishes. In particular, by Theorem 1.3, this means that $u\gamma$ vanishes itself almost everywhere and as γ is everywhere positive this means that u vanishes almost everywhere. This finishes the proof that $(H_n)_n$ is dense in $L^2(\mathbf{R}, \mathrm{d}\gamma)$. In conclusion we summarize this important result.

1.1 Proposition The Hermite polynomials $(H_n)_{n \in \mathbf{N}}$ are an orthogonal basis for $L^2(\mathbf{R}, \mathrm{d}\gamma)$.

Recalling the normalization (1.19)

$$h_n = \frac{H_n}{\sqrt{2^n n!}},$$

the coefficients in the expansion

$$u = \sum_{n=0}^{\infty} a_n h_n, \tag{1.21}$$

are then given by $a_n = \langle u, e_n \rangle$ where the convergence is in $L^2(\mathbf{R}, \mathrm{d}\gamma)$. To write this in the orthogonal basis $(H_n)_n$, all we need is use (1.19). So, for

(1.21) this gives

$$u = \sum_{n=0}^{\infty} \frac{\langle u, H_n \rangle}{n! 2^n} H_n.$$

These concepts are explained in greater detail in many standard functional analysis textbooks such as [2, 7, 9].

We have yet to introduce Hermite polynomials on $\mathbf{R}^d$, as of now, all computations we have done are for the case $d = 1$ only, whereas we defined the Gaussian measure (1.2) for all integer dimensions. This is the content of the next section.

1.2.4. Hermite polynomials on $\mathbf{R}^d$

In this section, we will define the Hermite polynomial H_α for a multiindex $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$ on $\mathbf{R}^d$. First we define the length $|\alpha|$ of α as

$$|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_d. \tag{1.22}$$

While the factorial $\alpha!$ is given by

$$\alpha! = \alpha_1! \alpha_2! \ldots \alpha_d! \tag{1.23}$$

Then we define H_α as

$$H_\alpha(x) = \bigotimes_{i=1}^{d} H_{\alpha_i}(x) = \prod_{i=1}^{d} H_{\alpha_i}(x_i).$$

Thus, the “higher order” Hermite polynomials are simple tensor products of the one-dimensional ones. Most of the identities for the higher order Hermite polynomials follow easily from the one-dimensional case.

As we are going to use the Hermite polynomials on $\mathbf{R}^d$, we still need to verify their density in $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ which can be done by bootstrapping the result in one dimension. We will do this through (1.20). Let $x = (x_1, \ldots, x_d)$ and $u \in L^2(\mathbf{R}^d, \mathrm{d}\gamma)$, then writing

$$\begin{aligned}\int_{\mathbf{R}^d} & H_\alpha(x) u(x)\,\mathrm{d}\gamma(x) \\ &= \underbrace{\int \cdots \int}_{d \text{ times}} \prod_{i=1}^{d} H_{\alpha_i}(x_i) u(x)\,\mathrm{d}\gamma(x_1)\,\mathrm{d}\gamma(x_2)\ldots\,\mathrm{d}\gamma(x_d) \\ &= \int_{\mathbf{R}} H_{\alpha_1}(x_1) \int_{\mathbf{R}} H_{\alpha_2}(x_2) \ldots \int_{\mathbf{R}} H_{\alpha_d}(x_d) u(x)\,\mathrm{d}\gamma(x).\end{aligned}$$

Assuming the integral on the left-hand side is zero for all α, we need to show that $u = 0$ almost everywhere. Note that from the one-dimensional case we know that

$$\int_{\mathbf{R}} H_{\alpha_d}(x_d) u(x_1, \ldots, x_d)\,\mathrm{d}\gamma(x_d) = 0,$$

hence $u = 0$ almost everywhere.

Similarly, we can use (1.19) to see that

$$\begin{aligned}\|H_\alpha\|^2_{L^2(\mathbf{R}^d, \mathrm{d}\gamma)} &= \prod_{i=1}^{d} \int_{\mathbf{R}^d} |H_{\alpha_i}(x_i)|^2\,\mathrm{d}\gamma(x) \\ &= \prod_{i=1}^{d} \frac{1}{2^{\alpha_i}\alpha_i!}.\end{aligned}$$

Recalling (1.22) and (1.23) we can see that the $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$ norm of H_α is given by

$$\|H_\alpha\|_{L^2(\mathbf{R}^d, \mathrm{d}\gamma)} = \frac{1}{\sqrt{2^{|\alpha|}\alpha!}}.$$

In the next section collects some additional identities related to the Hermite polynomials: A prototype question for instance is can we expand $H_n(x+y)$ in terms of $H_n(y)$?

1.2.5. Some identities

In this section we collect some identities related to the Hermite polynomials for $d=1$. In Chapter 3 we will make use of the expansion

$$H_n(x+y)=\sum_{k=0}^{n}\binom{n}{k}(2y)^{n-k}H_k(x). \tag{1.24}$$

We will prove this through the generating function (1.14). That is,

$$\begin{aligned} e^{2(x+y)t-t^2} &= \sum_{k=0}^{\infty}\frac{H_k(x+y)}{k!}t^k \\ &= \sum_{k=0}^{\infty}\frac{H_k(x)}{k!}t^k\sum_{n=0}^{\infty}\frac{(2yt)^n}{n!}. \end{aligned}$$

Rearranging the sum we see that

$$\sum_{k=0}^{\infty}\sum_{n=k}^{\infty}\frac{H_k(x)t^k}{k!}\frac{(2yt)^{n-k}}{(n-k)!}=\sum_{n=0}^{\infty}\frac{t^n}{n!}\sum_{k=0}^{n}\binom{k}{n}\frac{H_k(x)t^k}{k!}(2yt)^{n-k}.$$

Comparing coefficients in the power series we see that $H_k(x+y)$ and

$$\sum_{k=0}^{n}\binom{k}{n}\frac{H_k(x)t^k}{k!}(2yt)^{n-k}.$$

have the same generating function which proves (1.24).

A related question is concerns the product of Hermite polynomials. In particular, we look for the coefficients $(a_k^{m,n})$ in

$$H_m(x)H_n(x)=\sum_{k=0}^{m+n}a_k^{m,n}H_k(x). \tag{1.25}$$

To obtain these, we multiply both sides by $H_\ell(x)$, and use (1.13) to obtain

$$\int_{\mathbf{R}} H_m(x)H_n(x)H_\ell(x)\,\mathrm{d}\gamma(x) = \sum_{k=0}^{m+n} a_k^{m,n} \int_{\mathbf{R}} H_k(x)H_\ell(x)\,\mathrm{d}\gamma(x)$$
$$\overset{(1.25)}{=} 2^\ell \ell! \sum_{k=0}^{m+n} a_k^{m,n} \delta_{k,\ell}.$$

That is,

$$a_\ell^{m,n} = \frac{1}{\ell! 2^\ell} \int_{\mathbf{R}} H_m(x)H_n(x)H_\ell(x)\,\mathrm{d}\gamma(x). \tag{1.26}$$

To find the integral in (1.26) we use the generating function (1.14). That is

$$\begin{aligned}
&\int_{\mathbf{R}} \sum_{n,m,\ell=0}^{\infty} \frac{H_n(x)H_m(x)H_\ell(x)}{n!m!\ell!} r^n s^m t^\ell \,\mathrm{d}\gamma(x) \\
&= \int_{\mathbf{R}} \mathrm{e}^{2xr-r^2} \mathrm{e}^{2xs-s^2} \mathrm{e}^{2xt-t^2} \,\mathrm{d}\gamma(x) \\
&= \mathrm{e}^{2(rs+rt+st)} \int_{\mathbf{R}} \mathrm{e}^{-(x-r-s-t)^2} \frac{\mathrm{d}x}{\sqrt{\pi}} \\
&= \sum_{n,m,\ell=0}^{\infty} \frac{2^{n+m+\ell} r^{n+m} s^{n+\ell} t^{m+\ell}}{n!m!\ell!}.
\end{aligned}$$

Hence, comparing coefficients, we obtain $(a_k^{m,n})$ as in (1.25). That is

$$\begin{aligned}
a_\ell^{m,n} &= \frac{1}{\ell! 2^\ell} \int_{\mathbf{R}} H_m(x)H_n(x)H_\ell(x)\,\mathrm{d}\gamma(x) \\
&= \frac{2^{\frac{n+m-\ell}{2}} n! m!}{\left(\frac{\ell+m-n}{2}\right)! \left(\frac{m+n-\ell}{2}\right)! \left(\frac{n+\ell-m}{2}\right)!},
\end{aligned}$$

whenever $n+m+\ell$ is even and $n+m \geqslant \ell$, $n+\ell \geqslant n$ and $m+\ell \geqslant n$, and $a_\ell^{m,n} = 0$ in all other cases.

The next section explains the connection between the eigenfunctions of a Ornstein–Uhlenbeck operator and the Hermite polynomials.

1.3. Ornstein and Uhlenbeck

1.3.1. But first, some symmetry

In this section we investigate the relationship between the Hermite polynomials and the Ornstein–Uhlenbeck operator (1.5). We first proceed by unraveling some of the structure of the Ornstein–Uhlenbeck operator by introducing a so-called *bilinear form*. In the theory of Markov processes, bilinear forms play an important rôle, and the Ornstein–Uhlenbeck operator can also be associated to such a stochastic process[5]. As we work with the Gaussian measure (1.2), we will incorporate the Gaussian measure in the bilinear form. Additionally, this bilinear form is defined on a suitable class of *test functions* $\mathscr{D}$ which usually depends on the precise context, but we choose $\mathscr{D} = C_{\mathrm{c}}^{\infty}(\mathbf{R}^d)$ here. The canonical bilinear form $\mathscr{E}$ is

$$\mathscr{E}(u, v) := \int_{\mathbf{R}^d} \nabla u \cdot \nabla v \,\mathrm{d}\gamma,$$

Using (1.4) we can verify using integration by parts that the Ornstein–Uhlenbeck operator L satisfies the identity

$$\mathscr{E}(u, v) = \int_{\mathbf{R}^d} \nabla u \cdot \nabla v \,\mathrm{d}\gamma = \int_{\mathbf{R}^d} uLv \,\mathrm{d}\gamma. \tag{1.27}$$

In the next section we proceed with deriving some of the relations between the operator L and the polynomials $(H_n)_n$.

[5] In particular to a *Brownian motion* with drift or friction.

1.3.2. Ornstein, Uhlenbeck, Hermite and ... action!

As we have seen, we can decompose $L^2(\mathbf{R}, \mathrm{d}\gamma)$ as a direct sum of the subspaces $\mathscr{H}_n$ which each are defined as the closure of the linear span of a single Hermite polynomial H_n. Our purpose is to investigate what the action of L is on these subspaces.

We have an explicit description for the Ornstein–Uhlenbeck operator L and rather explicit definitions for the Hermite polynomials $(H_n)_n$, but we choose to proceed with the bilinear identity (1.27). Note that $\nabla = \partial_x$ and let $u = H_n$ and $v = H_m$. From (1.17) we see that $\nabla u = 2nH_{n-1}$ and $\nabla v = 2mH_{m-1}$. So, using these u and v in (1.27) we see that,

$$\int_{\mathbf{R}} H_n L H_m \,\mathrm{d}\gamma = 4nm \int_{\mathbf{R}} H_{n-1} H_{m-1} \,\mathrm{d}\gamma \overset{(1.13)}{=} 2^n n n! \delta_{nm}. \tag{1.28}$$

This implies for $n \neq m$ that H_n and LH_m are orthogonal. In particular, this means that LH_m is a scalar multiple c of H_m. The coefficient can now easily be deduced from (1.28). If we set $n = m$, we get

$$c2^n n! = 2^n n n! \text{ which implies } c = n.$$

So, we conclude that the Hermite polynomials (H_n) are *eigenfunctions* for L with *eigenvalue* n. That is

$$LH_n = nH_n \text{ for all } n \text{ in } \mathbf{N}. \tag{1.29}$$

As $H_0 = 1$ is the only Hermite polynomial with non-zero mean, we see that by applying the operator L to the Hermite expansion of a function u, the result will have mean zero.

As before, we can bootstrap (1.29) to the d-dimensional case. For this, let L_i be the Ornstein–Uhlenbeck operator with respect to the i^{th} variable.

Then $L = L_1 + \cdots + L_d$ and

$$\begin{aligned} L \bigotimes_{i=1}^{d} H_{\alpha_i} &= \sum_{j=1}^{d} L_j H_{\alpha_j} \bigotimes_{\substack{i=1 \\ i \neq j}}^{d} H_{\alpha_i} \\ &= \sum_{j=1}^{d} \alpha_j \bigotimes_{i=1}^{d} H_{\alpha_i} \\ &= |\alpha| \bigotimes_{i=1}^{d} H_{\alpha_i}. \end{aligned}$$

Hence,

$$LH_\alpha = |\alpha| H_\alpha \text{ for all } \alpha \text{ in } \mathbf{N}^d.$$

1.3.3. Mehler, Ornstein and Uhlenbeck

We define bounded operators $T(t) := \mathrm{e}^{tL}$ on $L^2(\mathbf{R}, \mathrm{d}\gamma)$ for $t \geqslant 0$ through their action on the Hermite polynomials $(H_n)_n$ by

$$\mathrm{e}^{tL} H_n = \mathrm{e}^{-nt} H_n,$$

and extend to $L^2(\mathbf{R}, \mathrm{d}\gamma)$ through linearity and density. We can the verify that the function $u(x,t) = \mathrm{e}^{tL} u_0(x)$ solves the *Abstract Cauchy Problem*, that is,

$$\begin{cases} \partial_t u &= Lu, \\ u(0) &= u_0. \end{cases}$$

The operators $\{T(t)\}_{t \geqslant 0}$ satisfy

1. For $t = 0$ we have $T(0) = 1$, the identity;

2. For each positive t and s we have

$$T(t+s) = T(t)T(s);$$

3. For each “initial value” u_0 we have the *convergence in the strong operator topology*, that is, we have

$$\|T(t)u_0 - u_0\| \to 0 \text{ as } t \downarrow 0.$$

These are the defining properties of a C_0-semigroup. The first and second properties state that the semigroup behaves like an exponential function. The third property states that the solution should depend continuously on t and starts at u_0.

The operators e^{tL} for $t \geqslant 0$ can be too complicated to handle when it comes down to computations with general functions without explicit Hermite basis expansion. In the next section, we will derive an integral kernel, the so-called *Mehler kernel*, for e^{tL} which will make the explicit computations as done in Chapters 2-4 easier to handle.

1.3.4. The Mehler kernel

The purpose of this section is to obtain a *Schwartz kernel* for the Ornstein–Uhlenbeck semigroup e^{tL}. That is, we seek for a function, which we denote by M_t after its namesake *Gustav Ferdinand Mehler* of two variables such that for all u in $L^2(\mathbf{R}, \mathrm{d}\gamma)$ and $t \geqslant 0$ we have

$$\mathrm{e}^{tL}u(x) = \int_{\mathbf{R}^d} M_t(x,y)u(y)\,\mathrm{d}\gamma(y). \tag{1.30}$$

As before, we expand write u in its Fourier-Hermite expansion (1.21) and use the boundedness of e^{tL} to see that

$$\mathrm{e}^{tL}u(x) = \mathrm{e}^{tL}\sum_{n=0}^{\infty} a_n h_n = \sum_{n=0}^{\infty} \mathrm{e}^{-nt} a_n h_n.$$

Recall that h_n is the normalized Hermite polynomial (1.19) and that $a_n = \langle u, h_n \rangle$. So,

$$\mathrm{e}^{tL}u(x) = \int_{\mathbf{R}^d} \sum_{n=0}^{\infty} \mathrm{e}^{-nt} h_n(x)h_n(y)u(y)\,\mathrm{d}\gamma(y).$$

Here, the inner sum

$$M_t(x,y) = \sum_{n=0}^{\infty} \mathrm{e}^{-nt} h_n(x)h_n(y), \tag{1.31}$$

is said to be the *Mehler kernel*. In what follows, we will also use the tensor notation

$$(h_n \otimes h_n)(x,y) = h_n(x)h_n(y).$$

An expression of the Mehler kernel as an infinite sum is often rather unsatisfactory and we will proceed by computing a closed form expression for M_t. We notice that M_t is symmetric in x and y, a fact which we will exploit in Chapter 2.

Proceeding, we will expand both Hermite polynomials in (1.31) using the integral expression (1.12) for H_n and the normalization (1.19). So,

$$h_n(x) = (-i)^n \sqrt{\frac{2^n}{n!}} \mathrm{e}^{x^2} \int_{\mathbf{R}} \xi^n \mathrm{e}^{2ix\xi}\, \mathrm{e}^{-\xi^2} \frac{\mathrm{d}\xi}{\sqrt{\pi}}.$$

Hence, substituting this expression into the series for M_t gives,

$$\begin{aligned}\sum_{n=0}^{\infty} \mathrm{e}^{-nt}(h_n \otimes h_n)(x,y) \\ = \mathrm{e}^{x^2+y^2} \int_{\mathbf{R}^2} \sum_{n=0}^{\infty} \frac{(-2\xi\eta e^{-t})^n}{n!} \mathrm{e}^{2i(x\xi+y\eta)} \mathrm{e}^{-\xi^2-\eta^2} \frac{\mathrm{d}\xi\,\mathrm{d}\eta}{\pi}.\end{aligned} \tag{1.32}$$

The series under the integral sign is the exponential, that is,

$$\sum_{n=0}^{\infty} \frac{(-2\xi\eta e^{-t})^n}{n!} = \mathrm{e}^{-2\xi\eta\mathrm{e}^{-t}}.$$

So, this reduces (1.32) to

$$\mathrm{e}^{x^2+y^2} \int_{\mathbf{R}^2} \mathrm{e}^{-2\xi\eta\mathrm{e}^{-t}} \mathrm{e}^{2i(x\xi+y\eta)} \mathrm{e}^{-\xi^2-\eta^2} \frac{\mathrm{d}\xi\,\mathrm{d}\eta}{\pi}.$$

Performing this integration gives

$$M_t(x,y) = \frac{1}{\sqrt{1-\mathrm{e}^{-2t}}} \exp\left(2\frac{xy}{\mathrm{e}^t+1}\right) \exp\left(-\frac{(x-y)^2}{\mathrm{e}^{2t}-1}\right).$$

In this dissertation, we will use the Mehler kernel on $\mathbf{R}^d$, and we can derive an expression for the Mehler kernel in $\mathbf{R}^d$ from the one-dimensional version. Note that is sufficient to test e^{tL} against a d-dimensional Hermite polynomial H_α. Recall that if we denote the one-dimensional Ornstein–Uhlenbeck operator with respect to the i^{th} variable by L_i we have that $L = L_1 + L_2 + \cdots + L_d$. As $L_i L_j = L_j L_i$ for all $i, j = 1, \ldots, d$ we then have

$$\mathrm{e}^{tL} = \prod_{i=1}^{d} \mathrm{e}^{tL_i},$$

hence,

$$\begin{aligned}
\mathrm{e}^{tL} h_\alpha(x) &= \mathrm{e}^{tL} \prod_{i=1}^{d} h_{\alpha_i}(x_i) \\
&= \prod_{i=1}^{d} \mathrm{e}^{tL_i} h_{\alpha_i}(x_i) \\
&= \prod_{i=1}^{d} \int_{\mathbf{R}} M_t^{(1)}(x_i, y_i) h_{\alpha_i}(y_i)\, \mathrm{d}\gamma(y_i),
\end{aligned}$$

where $M_t^{(1)}$ is the one-dimensional Mehler kernel. So, to obtain the d-dimensional version, we can take the simple tensor product of $M_t^{(1)}$. That is,

$$\begin{aligned}
M_t(x,y) &= \bigotimes_{i=1}^{d} M_t^{(1)}(x_i, y_i) \\
&= \frac{1}{(1-\mathrm{e}^{-2t})^{d/2}} \exp\left(2\frac{\langle x, y\rangle}{\mathrm{e}^t + 1}\right) \exp\left(-\frac{|x-y|^2}{\mathrm{e}^{2t}-1}\right).
\end{aligned} \tag{1.33}$$

1.4. There is also some uncertainty

A general principle from harmonic analysis is given in [5] and roughly states the following:

"A non-zero function cannot be sharply localized in both frequency and time."

We will proceed by following the idea of [1] and explain the relationship between the Hermite polynomials and the uncertainty principle. We will use a different Gaussian measure, and a scaling of the Hermite polynomials.

First, we set u_n to be the n^{th} *Hermite function*. That is, set

$$u_n(x) := \frac{1}{\sqrt{n!2^n}} H_n(x) \mathrm{e}^{-x^2/2}.$$

Then the n^{th} *De Bruijn-Hermite function* ψ_n is given by

$$\psi_n(x) := 2^{1/4} u_n(\sqrt{2\pi} x) = \frac{1}{\sqrt{n!2^{n-\frac{1}{2}}}} H_n(\sqrt{2\pi} x) \mathrm{e}^{-\pi x^2}.$$

Note that the orthogonality property (1.13) of the Hermite polynomials implies the orthogonality of (u_n) in $L^2(\mathbf{R})$. That is,

$$\begin{aligned} \frac{1}{\sqrt{\pi}} \int_{\mathbf{R}} u_n(\xi) u_m(\xi) \, \mathrm{d}\xi &= \sqrt{\frac{\pi}{n!m!2^{n+m}}} \int_{\mathbf{R}} H_n(\xi) H_m(\xi) \mathrm{e}^{-\xi^2} \, \gamma(\mathrm{d}\xi) \\ &\overset{(1.13)}{=} \delta_{nm}. \end{aligned} \tag{1.34}$$

By the substitution $\sqrt{2\pi}\xi \to \xi$, this implies the orthonormality for the De Bruijn-Hermite functions (ψ_n). That is,

$$\int_{\mathbf{R}} \psi_n(\xi) \psi_m(\xi) \, \mathrm{d}\xi \overset{(1.34)}{=} \delta_{nm}.$$

We will also require the Fourier transform $\widehat{\psi_n}$ of ψ_n. For this, we compute $\widehat{u}_n$. That is, we wish to find

$$\widehat{u}_n(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} u_n(\xi) \mathrm{e}^{-ix\xi} \, \mathrm{d}\xi = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} H_n(\xi) \mathrm{e}^{-\xi^2/2} \mathrm{e}^{-ix\xi} \, \mathrm{d}\xi. \tag{1.35}$$

Next, we use the Rodrigues's formula (1.11) as a representation of H_n in (1.35) to get

$$\begin{aligned} \widehat{u}_n(x) &= \frac{(-1)^n}{\sqrt{2\pi}} \int_{\mathbf{R}} \mathrm{e}^{\xi^2/2} \mathrm{e}^{-ix\xi} \partial_\xi^n \mathrm{e}^{-\xi^2} \, \mathrm{d}\xi \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} \mathrm{e}^{-\xi^2} \partial_\xi^n \mathrm{e}^{-ix\xi + \xi^2/2} \, \mathrm{d}\xi. \end{aligned}$$

Completing the square gives

$$\begin{aligned}\widehat{u}_n(x) &= \frac{e^{x^2/2}}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{-\xi^2} \partial_\xi^n e^{(\xi - ix)^2/2}\, d\xi \\ &= (-1)^n i^n \frac{e^{x^2/2}}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{-\xi^2} \partial_x^n e^{(\xi + ix)^2/2}\, d\xi.\end{aligned}$$

Next, (1.8) allows us to find the integral on the right-hand side, that is,

$$\begin{aligned}\frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{-\xi^2} \partial_x^n e^{(\xi+ix)^2/2}\, d\xi &= \frac{1}{\sqrt{2\pi}} \partial_x^n \int_{\mathbf{R}} e^{-\xi^2} e^{(\xi+ix)^2/2}\, d\xi \\ &\overset{(1.8)}{=} \partial_x^n e^{-x^2}.\end{aligned}$$

We conclude by virtue of the Rodrigues formula (1.11) that

$$\widehat{u}_n(x) = (-1)^n i^n e^{x^2/2} \partial_x^n e^{-x^2} \overset{(1.11)}{=} i^n e^{-x^2/2} H_n(x) = i^n u_n(x).$$

A substitution directly shows that $\widehat{\psi_n}$ satisfies the eigenvalue equation

$$\widehat{\psi_n} = i^n \psi_n. \tag{1.36}$$

We have all the ingredients in place to prove the uncertainty principle using the basis (ψ_n). For this, let u be in $L^2(\mathbf{R}, d\gamma)$ and let $\widehat{u}$ in $L^2(\mathbf{R}, d\gamma)$ be its Fourier-Plancherel transform. The orthogonality (1.34) together with the Hermite expansion (1.21) allows us to represent $x \mapsto u(x)$ and $x \mapsto xu(x)$ in the basis (ψ_n). In particular, we have,

$$u(x) = \sum_{n=0}^{\infty} a_n \psi_n(x), \tag{1.37}$$

$$xu(x) = \sum_{n=0}^{\infty} b_n \psi_n(x). \tag{1.38}$$

We use (1.36) to find $\widehat{u}$, that is,

$$\widehat{u}(x) = \sum_{n=0}^{\infty} a_n i^n \psi_n(x),$$
$$x\widehat{u}(x) = \sum_{n=0}^{\infty} c_n \psi_n(x).$$

Next, we will give a recursion relation between the coefficients (a_n), (b_n) and (c_n). To do this we first recall the recursion relation (1.18) for the

$$2xH_n(x) = H_{n+1}(x) - 2nH_{n-1}(x).$$

For the De Bruijn-Hermite functions this gives the recursion

$$\sqrt{4\pi}x\psi_n(x) = \sqrt{n+1}\psi_{n+1}(x) + \sqrt{n}\psi_{n-1}(x). \tag{1.39}$$

The connection between (a_n) and (b_n) is easy, using (1.39) we obtain

$$\sqrt{4\pi}b_n = \sqrt{n+1}a_n + \sqrt{n}a_{n-1}. \tag{1.40}$$

For (a_n) and (c_n) we have by (1.39) that

$$\sqrt{4\pi}c_n = (-1)^{n+1} i^{n+1} [\sqrt{n+1}a_n + \sqrt{n}a_{n-1}]. \tag{1.41}$$

Hence, we can compute the variances (1.37) and (1.38) of u and $\widehat{u}$. Let us first determine $|b_n|^2$ and $|c_n|^2$ from (1.40) and (1.41). That is,

$$\begin{aligned}|b_n|^2 &= \frac{1}{4\pi}\left|\sqrt{n+1}a_n + \sqrt{n}a_{n-1}\right|^2 \\ &= \frac{1}{4\pi}\left[(n+1)|a_n|^2 + n|a_{n-1}|^2 + 2\sqrt{n(n+1)}\operatorname{Re}\overline{a_n}a_{n-1}\right].\end{aligned}$$

And $|c_n|^2$ is

$$\begin{aligned}|c_n|^2 &= \frac{1}{4\pi}\left|\sqrt{n+1}a_n - \sqrt{n}a_{n-1}\right|^2 \\ &= \frac{1}{4\pi}\left[(n+1)|a_n|^2 + n|a_{n-1}|^2 - 2\sqrt{n(n+1)}\operatorname{Re}\overline{a_n}a_{n-1}\right].\end{aligned}$$

Hence, we have by Parseval's identity that

$$\int_{-\infty}^{\infty} x^2|u(x)|^2\,\mathrm{d}x + \int_{-\infty}^{\infty} \xi^2|\widehat{u}(\xi)|^2\,\mathrm{d}\xi$$
$$= \frac{1}{4\pi}\left\{\sum_{n=0}^{\infty}\left[(n+1)|a_n|^2 + n|a_{n-1}|^2\right]\right\}$$
$$= \frac{1}{4\pi}\sum_{n=0}^{\infty} 2(n+1)|a_n|^2.$$

While, we have for the L^2 norm of u,

$$\int_{-\infty}^{\infty} |u(x)|^2\,\mathrm{d}x = \sum_{n=0}^{\infty}|a_n|^2.$$

So we have

$$\frac{1}{4\pi}\sum_{n=0}^{\infty} 2(n+1)|a_n|^2 \geqslant \frac{1}{2\pi}\sum_{n=0}^{\infty}|a_n|^2. \tag{1.42}$$

We have equality in (1.42) if and only if $a_n = 0$ for all $n \neq 0$. a_0 corresponds to the coefficient in (1.37). Recall that ψ_0 is given by

$$\psi_0(x) = 2^{\frac{1}{4}}\mathrm{e}^{-\pi x^2}.$$

This implies,

$$\int_{-\infty}^{\infty} x^2|u(x)|^2\,\mathrm{d}x + \int_{-\infty}^{\infty} \xi^2|\widehat{u}(\xi)|^2\,\mathrm{d}\xi \geqslant \frac{1}{2\pi}\int_{-\infty}^{\infty}|u(x)|^2\,\mathrm{d}x,$$

with equality if and only if u almost everywhere equal to $\exp(-\pi x^2)$ up to a multiplicative constant. Substituting x to xp^{-1} for some positive constant p gives,

$$p^2\int_{-\infty}^{\infty} x^2|u(x)|^2\,\mathrm{d}x + p^{-2}\int_{-\infty}^{\infty} \xi^2|\widehat{u}(\xi)|^2\,\mathrm{d}\xi \geqslant \frac{1}{2\pi}\int_{-\infty}^{\infty}|u(x)|^2\,\mathrm{d}x. \tag{1.43}$$

To find the sharpest inequality, we find p such that the left-hand side is minimal, as in the proof of Hölder's inequality. If we assume that $\|u\|_{L^2(\mathbf{R})} = 1$, which we can do without loss of generality by scaling, we can note that the two integrals on the left-hand side are the variances $\operatorname{Var} u$ and $\operatorname{Var} \widehat{u}$ of u and $\widehat{u}$ respectively. So, write the left-hand side as

$$p^2 \operatorname{Var} u + p^{-2} \operatorname{Var} \widehat{u}.$$

Computing the derivative with respect to p and setting equal to 0 shows that the minimum is attained at

$$p = \left(\frac{\operatorname{Var} \widehat{u}}{\operatorname{Var} u}\right)^{\frac{1}{4}}.$$

So, substituted in (1.43) this gives the uncertainty principle.

$$\left(\int_{-\infty}^{\infty} x^2 |u(x)|^2 \,\mathrm{d}x\right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} \xi^2 |\widehat{u}(\xi)|^2 \,\mathrm{d}\xi\right)^{\frac{1}{2}} \geqslant \frac{1}{4\pi} \int_{-\infty}^{\infty} |u(x)|^2 \,\mathrm{d}x.$$

1.5. A collection of useful results

This section collects some results are used in the main text, but would distract too much from the main content when these would be added there.

The first of such results is taken from [4], and uses the *Lebesgue dominated convergence theorem* to give conditions under which one can interchange integration and differentiation.

1.2 Theorem [4, Theorem 2.27] Let X be a measurable space and let $u : X \times (a, b) \to \mathbf{C}$ $(-\infty < a < b < \infty)$ be such that $u(\cdot, t) : X \to \mathbf{C}$ is integrable each t in (a,b). Let μ be a σ-finite measure, and set

$$U(t) = \int_X u(x,t)\,\mathrm{d}\mu(x).$$

Suppose that

1. $t \mapsto u(x,t)$ is differentiable for each x in X,
2. There is a v in $L^1(\mu)$ such that

$$|\partial_t u(x,t)| \leqslant v(x) \quad \text{for all } x \text{ and } t.$$

Then U is differentiable on (a,b) and,

$$U'(t) = \int_X \partial_t u(x,t)\,\mathrm{d}\mu(x).$$

Finally, the next theorem is particularily useful to conclude that if the Fourier transform of a function vanishes, the function itself must.

1.3 Theorem [4, Theorem 8.26] If $u \in L^1$ and $\widehat{u} = 0$, then $u = 0$ almost everywhere.

Further reading

The classical papers on the material in this chapter are [10, 11], while the book [6] puts the matter in a broader infinite dimensional perspective.

Furthermore, there is a large abundance of research on combinatorial interpretations of the Hermite polynomials. As far as Hermite polynomials are concerned [3] is a classic.

References

[1] N. G. de Bruijn. *Uncertainty principles in Fourier analysis*. Academic Press, New York, 1967, 57–71 (see pp. 4, 27).

[2] John B. Conway. *A course in functional analysis. 2nd ed.* English. 2nd ed. New York etc.: Springer-Verlag, 1990, xvi + 399 (see pp. 7, 17).

[3] Dominique Foata. "Some Hermite polynomial identities and their combinatorics". In: *Advances in Applied Mathematics* 2.3 (Sept. 1981), 250–259. DOI: 10.1016/0196-8858(81)90006-3 (see p. 33).

[4] Gerald B. Folland. *Real analysis*. Second Edition. Pure and Applied Mathematics (New York). Modern techniques and their applications, A Wiley-Interscience Publication. John Wiley & Sons, Inc., New York, 1999, xvi+386 (see pp. 32, 33).

[5] Gerald B. Folland and Alladi Sitaram. "The uncertainty principle: A mathematical survey". In: *The Journal of Fourier Analysis and Applications* 3.3 (May 1997), 207–238. DOI: 10.1007/BF02649110 (see p. 27).

[6] Svante Janson. *Gaussian Hilbert spaces*. English. Cambridge: Cambridge University Press, 1997, x + 340. DOI: 10.1017/CBO9780511526169 (see p. 33).

[7] Erwin Kreyzig. *Introductory Functional Analysis with Applications*. Wiley, 1978 (see p. 17).

[8] Giancarlo Mauceri and Stefano Meda. "BMO and H^1 for the Ornstein–Uhlenbeck operator". In: *Journal of Functional Analysis* 252.1 (Nov. 2007), 278–313. DOI: 10.1016/j.jfa.2007.06.017 (see p. 6).

[9] Walter Rudin. *Functional analysis*. Second. International Series in Pure and Applied Mathematics. McGraw-Hill, Inc., New York, 1991, xviii+424 (see pp. 7, 17).

[10] Peter Sjögren. "Operators associated with the Hermite semigroup—a survey". In: *J. Fourier Anal. Appl.* 3.Special Issue (1997), 813–823. DOI: 10.1007/BF02656487 (see p. 33).

[11] Sundaram Thangavelu. *Lectures on Hermite and Laguerre expansions*. Mathematical Notes. With a preface by Robert S. Strichartz. Princeton University Press, Princeton, NJ, 1993, xviii+195 (see p. 33).

2. The non-tangential Gaussian maximal functions

This note presents a proof that the non-tangential maximal function of the Ornstein–Uhlenbeck semigroup is bounded pointwise by the Gaussian Hardy–Littlewood maximal function. In particular this entails an extension on a result by Pineda and Urbina [5] who proved a similar result for a 'truncated' version with fixed parameters of the non-tangential maximal function. We actually obtain boundedness of the maximal function on non-tangential cones of arbitrary aperture.

This chapter has been published in Indagationes Mathematicae 26 (2015) 106-112 [10].

2.1. Introduction

Maximal functions are among the most studied objects in harmonic analysis. It is well-known that the classical non-tangential maximal function associated with the heat semigroup is bounded pointwise by the Hardy-Littlewood maximal function, for every $x \in \mathbf{R}^d$, i.e.,

$$\sup_{\substack{(y,t)\in\mathbf{R}^{d+1}_+\\|x-y|<t}} |\mathrm{e}^{t^2\Delta}u(y)| \lesssim \sup_{r>0} \frac{1}{|B_r(x)|}\int_{B_r(x)} |u|\,\mathrm{d}\lambda, \tag{2.1}$$

for all locally integrable functions u on $\mathbf{R}^d$ where λ is the Lebesgue measure on $\mathbf{R}^d$ (cf. [9, Proposition II 2.1.]). Here the action of *heat semigroup* $\mathrm{e}^{t\Delta}u = \rho_t * u$ is given by a convolution of u with the *heat kernel*

$$\rho_t(\xi) := \frac{\mathrm{e}^{-|\xi|^2/4t}}{(4\pi t)^{\frac{d}{2}}}, \text{ with } t > 0 \text{ and } \xi \in \mathbf{R}^d.$$

In this note we are interested in its Gaussian counterpart. The change from Lebesgue measure to the *Gaussian measure* (1.2) introduces quite some intricate technical and conceptual difficulties which are due to its non-doubling nature. Instead of the Laplacian, we will use its Gaussian analogue (1.6), the *Ornstein-Uhlenbeck operator* L which is given by

$$L := \frac{1}{2}\Delta - \langle x, \nabla\rangle = -\frac{1}{2}\nabla^*\nabla,$$

where ∇^* denotes the adjoint of ∇ with respect to the measure $\mathrm{d}\gamma$. Our main result, to be proved in Theorem 2.5, is the following Gaussian analogue of (2.1):

$$\sup_{(y,t)\in\Gamma_x^{(A,a)}} |\mathrm{e}^{t^2L}u(y)| \lesssim \sup_{r>0} \frac{1}{\gamma(B_r(x))}\int_{B_r(x)} |u|\,\mathrm{d}\gamma. \tag{2.2}$$

Here,

$$\Gamma_x^{(A,a)} := \Gamma_x^{(A,a)}(\gamma) := \{(y,t) \in \mathbf{R}_+^{d+1} \ : \ |x-y| < At \text{ and } t \leqslant am(x)\}$$

is the *Gaussian cone* with aperture A and cut-off parameter a, and

$$m(x) := \min\left\{1, \frac{1}{|x|}\right\}. \tag{2.3}$$

As shown in [3, Theorem 2.19] the centered Gaussian Hardy-Littlewood maximal function is of weak-type $(1,1)$ and is $L^p(\gamma)$-bounded for $1 < p \leqslant \infty$. In fact, the same result holds when the Gaussian measure γ is replaced by any Radon measure μ. Furthermore, if μ is doubling, then these results even hold for the *uncentered* Hardy-Littlewood maximal function. For the Gaussian measure γ the uncentered weak-type $(1,1)$ result is known to fail for $d > 1$ [7]. Nevertheless, the uncentered Hardy-Littlewood maximal function for γ is L^p-bounded for $1 < p \leqslant \infty$ [1].

A slightly weaker version of the inequality (2.2) has been proved by Pineda and Urbina [5] who showed that

$$\sup_{(y,t)\in\widetilde{\Gamma}_x} |\mathrm{e}^{t^2 L} u(y)| \lesssim \sup_{r>0} \frac{1}{\gamma(B_r(x))} \int_{B_r(x)} |u| \, \mathrm{d}\gamma,$$

where

$$\widetilde{\Gamma}_x = \{(y,t) \in \mathbf{R}_+^d : |x-y| < t \leqslant \widetilde{m}(x)\}$$

is the 'reduced' Gaussian cone corresponding to the function

$$\widetilde{m}(x) = \min\left\{\frac{1}{2}, \frac{1}{|x|}\right\}.$$

Our proof of (2.2) is shorter than the one presented in [5]. It has the further advantage of allowing the extension to cones with arbitrary aperture $A > 0$

and cut-off parameter $a > 0$ without any additional technicalities. This additional generality is important and has already been used by Portal (cf. the claim made in [6, discussion preceding Lemma 2.3]) to prove the H^1-boundedness of the Riesz transform associated with L.

2.2. The Mehler kernel

The *Mehler kernel* (see e.g., [8] and (1.30)) is the Schwartz kernel associated to the Ornstein-Uhlenbeck semigroup $(\mathrm{e}^{tL})_{t\geqslant 0}$, that is,

$$\mathrm{e}^{tL}u(x) = \int_{\mathbf{R}^d} M_t(x,\cdot)u \, \mathrm{d}\gamma.$$

There is an abundance of literature on the Mehler kernel and its properties. We shall only use the fact, proved e.g. in the survey paper [8], that it is given explicitly by

$$M_t(x,y) = \frac{\exp\left(-\frac{|\mathrm{e}^{-t}x-y|^2}{1-\mathrm{e}^{-2t}}\right)}{(1-\mathrm{e}^{-2t})^{\frac{d}{2}}}\mathrm{e}^{|y|^2}. \tag{2.4}$$

Note that the symmetry of the semigroup e^{tL} allows us to conclude that $M_t(x,y)$ is symmetric in x and y as well. A formula for (2.4) honoring this observation is given in (1.33):

$$M_t(x,y) = \frac{\exp\left(-\mathrm{e}^{-2t}\frac{|x-y|^2}{1-\mathrm{e}^{-2t}}\right)}{(1-\mathrm{e}^{-t})^{\frac{d}{2}}}\frac{\exp\left(2\mathrm{e}^{-t}\frac{\langle x,y\rangle}{1+\mathrm{e}^{-t}}\right)}{(1+\mathrm{e}^{-t})^{\frac{d}{2}}}. \tag{2.5}$$

2.3. Some lemmata

We use m as defined in (2.3) in our next lemma, which is taken from [2, Lemma 2.3].

2.1 Lemma Let a, A be strictly positive real numbers and $t > 0$. We have for $x, y \in \mathbf{R}^d$ that:

1. If $|x - y| < At$ and $t \leqslant am(x)$, then $t \leqslant a(1 + aA)m(y)$,
2. If $|x - y| < Am(x)$, then $m(x) \leqslant (1 + A)m(y)$ and $m(y) \leqslant 2(1 + A)m(x)$.

The next lemma, taken from [4, Proposition 2.1(i)], will come useful when we want to cancel exponential growth in one variable with exponential decay in the other as long both variables are in a Gaussian cone. For the reader's convenience, we include a short proof.

2.2 Lemma Let $\alpha > 0$ and $|x - y| \leqslant \alpha m(x)$. Then:

$$\mathrm{e}^{-\alpha^2 - 2\alpha} \mathrm{e}^{|y|^2} \leqslant \mathrm{e}^{|x|^2} \leqslant \mathrm{e}^{\alpha^2(1+\alpha)^2 + 2\alpha(1+\alpha)} \mathrm{e}^{|y|^2}.$$

Proof. By the triangle inequality and $m(x)|x| \leqslant 1$ we get,

$$|y|^2 \leqslant (\alpha m(x) + |x|)^2 \leqslant \alpha^2 + 2\alpha + |x|^2.$$

This gives the first inequality. For the second we use Lemma 2.1 to infer $m(x) \leqslant (1 + \alpha)m(y)$. Proceeding as before we obtain

$$|x|^2 \leqslant \alpha^2(1 + \alpha)^2 + 2\alpha(1 + \alpha) + |y|^2,$$

which finishes the proof. ∎

2.3.1. An estimate on Gaussian balls

Let $B := B_t(x)$ be the open Euclidean ball with radius t and center x and let γ be the Gaussian measure as defined by (1.2). We shall denote by S_d the surface area of the unit sphere in $\mathbf{R}^d$.

2.3 Lemma For all $x \in \mathbf{R}^d$ and $t > 0$ we have the inequality:

$$\gamma(B_t(x)) \leqslant \frac{S_d}{\pi^{\frac{d}{2}}} \frac{t^d}{d} \mathrm{e}^{2t|x|} \mathrm{e}^{-|x|^2}.$$

Proof. Remark that, with $B := B_t(x)$,

$$\begin{aligned}
\int_B \mathrm{e}^{-|\xi|^2}\, \mathrm{d}\xi &= \mathrm{e}^{-|x|^2} \int_B \mathrm{e}^{-|\xi-x|^2} \mathrm{e}^{-2\langle x, \xi - x\rangle}\, \mathrm{d}\xi \\
&\leqslant \mathrm{e}^{-|x|^2} \int_B \mathrm{e}^{-|\xi-x|^2} \mathrm{e}^{2|x||\xi-x|}\, \mathrm{d}\xi \\
&\leqslant \mathrm{e}^{-|x|^2} \mathrm{e}^{2t|x|} \int_B \mathrm{e}^{-|\xi-x|^2}\, \mathrm{d}\xi \\
&= \pi^{\frac{d}{2}} \mathrm{e}^{2t|x|} \mathrm{e}^{-|x|^2} \gamma(B_t(0)).
\end{aligned}$$

So, there holds that

$$\gamma(B_t(x)) \leqslant \mathrm{e}^{2t|x|} \mathrm{e}^{-|x|^2} \gamma(B_t(0)).$$

We proceed by noting that

$$\gamma(B_t(0)) \leqslant \pi^{-\frac{d}{2}} |B_t(0)| \leqslant \pi^{-\frac{d}{2}} t^d \frac{S_d}{d},$$

and combine this with the previous calculation to obtain

$$\gamma(B_t(x)) \leqslant \frac{S_d}{\pi^{\frac{d}{2}}} \frac{t^d}{d} \mathrm{e}^{2t|x|} \mathrm{e}^{-|x|^2}.$$

This completes the proof. ■

2.3.2. Off-diagonal kernel estimates on annuli

As is common in harmonic analysis, we often wish to decompose $\mathbf{R}^d$ into sets on which certain phenomena are easier to handle. Here we will decompose the space into disjoint annuli.

Throughout this subsection we fix $x \in \mathbf{R}^d$, constants $A, a \geqslant 1$, and a pair $(y,t) \in \Gamma_x^{(A,a)}$. We use the notation rB to mean the ball obtained from the ball B by multiplying its radius by r.

The annuli $C_k := C_k(B_t(y))$ are given by:

$$C_k := \begin{cases} 2B_t(y), & k = 0, \\ 2^{k+1}B_t(y) \setminus 2^k B_t(y), & k \geqslant 1. \end{cases} \tag{2.6}$$

So, whenever ξ is in C_k, we get for $k \geqslant 1$ that

$$2^k t \leqslant |y - \xi| < 2^{k+1} t. \tag{2.7}$$

On C_k we have the following bound for $M_{t^2}(y, \cdot)$:

2.4 Lemma For all $\xi \in C_k$ for $k \geqslant 1$ we have:

$$M_{t^2}(y,\xi) \leqslant \frac{\mathrm{e}^{|y|^2}}{(1-\mathrm{e}^{-2t^2})^{\frac{d}{2}}} \exp\big(2^{k+1} t|y|\big) \exp\Big(-\frac{4^k}{2\mathrm{e}^{2t^2}}\Big). \tag{2.8}$$

Proof. Considering the first exponential which occurs in the Mehler kernel (2.5) together with (2.7) gives for $k \geqslant 1$:

$$\begin{aligned} \exp\Big(-\mathrm{e}^{-2t^2} \frac{|y-\xi|^2}{1-\mathrm{e}^{-2t^2}}\Big) &\leqslant \exp\Big(-\frac{4^k}{\mathrm{e}^{2t^2}} \frac{t^2}{1-\mathrm{e}^{-2t^2}}\Big) \\ &\overset{(\dagger)}{\leqslant} \exp\Big(-\frac{4^k}{2\mathrm{e}^{2t^2}}\Big), \end{aligned}$$

where $(\dagger)$ follows from $1-\mathrm{e}^{-s} \leqslant s$ for $s \geqslant 0$. Using the estimate $1+s \geqslant 2s$ for $0 \leqslant s \leqslant 1$, we find for the second exponential in the Mehler kernel (2.5), by (2.7) that

$$\exp\Big(2\mathrm{e}^{-t^2}\frac{\langle y,\xi\rangle}{1+\mathrm{e}^{-t^2}}\Big) \leqslant \exp(|\langle y,\xi\rangle|)$$
$$\leqslant \exp(|\langle y,\xi-y\rangle|)\mathrm{e}^{|y|^2}$$
$$\leqslant \exp\big(2^{k+1}t|y|\big)\mathrm{e}^{|y|^2}.$$

Combining these estimates we obtain (2.8), as required. ∎

2.4. The main result

In this section we will prove our main theorem as mentioned in (2.2) for which the necessary preparations have already been made.

2.5 Theorem Let $A, a > 0$. For all $x \in \mathbf{R}^d$ and all $u \in C_c^\infty(\mathbf{R}^d)$ we have

$$\sup_{(y,t)\in\Gamma_x^{(A,a)}} |\mathrm{e}^{t^2L}u(y)| \lesssim \sup_{r>0} \frac{1}{\gamma(B_r(x))} \int_{B_r(x)} |u| \,\mathrm{d}\gamma, \tag{2.9}$$

where the implicit constant only depends on A, a and d.

Proof. We fix $x \in \mathbf{R}^d$ and $(y,t) \in \Gamma_x^{(A,a)}$. The proof of (2.9) is based on splitting the integration domain into the annuli C_k as defined by (2.6) and estimating on each annulus. Explicitly,

$$|\mathrm{e}^{t^2L}u(y)| \leqslant \sum_{k=0}^{\infty} I_k(y), \text{ where } I_k(y) := \int_{C_k} M_{t^2}(y,\cdot)|u(\cdot)| \,\mathrm{d}\gamma. \tag{2.10}$$

We have $t \leqslant am(x) \leqslant a$ and, by Lemma 2.1, $t|y| \leqslant a(1+aA)$. Together with Lemma 2.4 we infer, for $\xi \in C_k$ and $k \geqslant 1$, that

$$M_{t^2}(y,\xi) \leqslant \frac{\mathrm{e}^{|y|^2}}{(1-\mathrm{e}^{-2t^2})^{\frac{d}{2}}} \exp(2^{k+1}a(1+aA)) \exp\Big(-\frac{4^k}{2\mathrm{e}^{2a^2}}\Big)$$
$$=: \frac{\mathrm{e}^{|y|^2}}{(1-\mathrm{e}^{-2t^2})^{\frac{d}{2}}} c_k.$$

Combining this with Lemma 2.2, we obtain

$$M_{t^2}(y,\xi) \lesssim_{A,a} \frac{e^{|x|^2}}{(1-e^{-2t^2})^{\frac{d}{2}}} c_k. \tag{2.11}$$

Also, by (2.7) we get

$$|x-\xi| \leqslant |x-y| + |\xi - y| \leqslant (2^{k+1}+A)t.$$

Let K be the smallest integer such that $2^{k+1} \geqslant A$ whenever $k \geqslant K$. Then it follows that C_k for $k \geqslant K$ is contained in $B_{2^{k+2}t}(x)$ and for $k < K$ is contained in $B_{2At}(x)$. We set

$$D_k := D_k(x) = \begin{cases} B_{2^{k+2}t}(x) & \text{if } k \geqslant K, \\ B_{2At}(x) & \text{elsewhere.} \end{cases}$$

Let us denote the supremum on right-hand side of (2.9) by $M_\gamma u(x)$. Using (2.11), we can bound the integral on the right-hand side of (2.10) by

$$\begin{aligned} \int_{C_k} M_{t^2}(y,\cdot)|u(\cdot)| \, d\gamma &\lesssim_{A,a} c_k \frac{e^{|x|^2}}{(1-e^{-2t^2})^{\frac{d}{2}}} \int_{C_k} |u| \, d\gamma \\ &\leqslant c_k \frac{e^{|x|^2}}{(1-e^{-2t^2})^{\frac{d}{2}}} \int_{D_k} |u| \, d\gamma \\ &\leqslant c_k \frac{e^{|x|^2}}{(1-e^{-2t^2})^{\frac{d}{2}}} \gamma(D_k) M_\gamma u(x), \end{aligned}$$

where we pause for a moment to compute a suitable bound for $\gamma(D_k)$. As above we have both $t|x| \leqslant am(x)|x| \leqslant a$ and $t \leqslant a$. Together with Lemma 2.3 applied to D_k for $k \geqslant K$ we obtain:

$$\begin{aligned} \gamma(D_k) e^{|x|^2} &\lesssim_A C^d \frac{S_d}{d} t^d 2^{kd} e^{2^{k+3} t|x|} e^{-|x|^2} e^{|x|^2} \\ &\lesssim_{A,a,d} t^d 2^{kd} e^{2^{k+3} a}. \end{aligned}$$

Similarly, for $k < K$:

$$\gamma(D_k)\mathrm{e}^{|x|^2} \lesssim_{A,a,d} t^d \mathrm{e}^{2Aa}.$$

Using the bound $t \leqslant a$, we can infer that

$$\frac{t^d}{(1-\mathrm{e}^{-2t^2})^{\frac{d}{2}}} \leqslant \frac{a^d}{(1-\mathrm{e}^{-2a^2})^{\frac{d}{2}}} \lesssim_{a,d} 1.$$

(note that $s/(1-\mathrm{e}^{-s})$ is increasing). Combining these computations with the ones above for $k \geqslant K$ we get

$$\int_{C_k} M_{t^2}(y,\cdot)|u(\cdot)|\,\mathrm{d}\gamma \lesssim_{A,a,d} c_k 2^{kd} \mathrm{e}^{2^{k+2}a} M_\gamma u(x),$$

while for $k < K$ we get

$$\int_{C_k} M_{t^2}(y,\cdot)|u(\cdot)|\,\mathrm{d}\gamma \lesssim_{A,a,d} c_k M_\gamma u(x).$$

Similarly, for $\xi \in 2B_t(x)$ we obtain:

$$I_0 := \int_{2B_t} M_{t^2}(y,\cdot)|u(\cdot)|\,\mathrm{d}\gamma \lesssim_{A,a,d} M_\gamma u(x).$$

Inserting the dependency of c_k upon k as coming from (2.11), we obtain the bound:

$$\begin{aligned}
|\mathrm{e}^{t^2L}u(y)| &= I_0 + \sum_{k=1}^{K-1} I_k + \sum_{k=K}^{\infty} I_k \\
&\lesssim_{A,a,d} \left[1 + \sum_{k=1}^{K-1} c_k + \sum_{k=K}^{\infty} c_k 2^{kd} \mathrm{e}^{2^{k+2}a}\right] M_\gamma u(x), \\
&\lesssim_{A,a,d} \left[1 + \sum_{k=1}^{K-1} \mathrm{e}^{-\frac{4^k}{2\mathrm{e}^{2a^2}}} + \sum_{k=K}^{\infty} 2^{kd} \mathrm{e}^{2^{k+1}(1+2a+aA)} \mathrm{e}^{-\frac{4^k}{2\mathrm{e}^{2a^2}}}\right] M_\gamma u(x),
\end{aligned}$$

valid for all $(y,t) \in \Gamma_x^{(A,a)}$. As the sum on the right-hand side evidently converges, we see that taking the supremum proves (2.9). ■

2.5. Acknowledgments

This work initiated as part of a larger project in collaboration with Mikko Kemppainen. I would like to thank the referee for his/her useful suggestions.

References

[1] L. Forzani et al. "On the L^p boundedness of the non-centered Gaussian Hardy-Littlewood maximal function". In: *Proceedings of the American Mathematical Society* 130.1 (2002), 73–79. DOI: 10.1090/S0002-9939-01-06156-1 (see p. 39).

[2] Jan Maas, Jan van Neerven, and Pierre Portal. "Whitney coverings and the tent spaces $T^{1,q}(\gamma)$ for the Gaussian measure". In: *Arkiv för Matematik* 50.2 (Apr. 2011), 379–395. DOI: 10.1007/s11512-010-0143-z (see p. 41).

[3] Pertti Mattila. *Geometry of Sets and Measures in Euclidean Spaces*. Cambridge: Cambridge University Press, 1995. DOI: 10.1017/CBO9780511623813 (see p. 39).

[4] Giancarlo Mauceri and Stefano Meda. "BMO and H^1 for the Ornstein–Uhlenbeck operator". In: *Journal of Functional Analysis* 252.1 (Nov. 2007), 278–313. DOI: 10.1016/j.jfa.2007.06.017 (see p. 41).

[5] Ebner Pineda and Wilfredo Urbina R. "Non tangential convergence for the Ornstein-Uhlenbeck semigroup". In: *Divulgaciones Matematicas* 16.2 (2008), 107–124. arXiv: 0611040 [math] (see pp. 37, 39).

[6] Pierre Portal. "Maximal and quadratic gaussian Hardy spaces". In: *Revista Matematica Iberoamericana* 30 (Mar. 2014), 79–108. DOI: 10.4171/rmi/770. arXiv: 1203.1998 (see p. 40).

[7] Peter Sjögren. "A Remark on the Maximal Function for Measures in $\mathbf{R}^n$". In: *American Journal of Mathematics* 105.5 (Oct. 1983), 1231–1233. DOI: 10.2307/2374340 (see p. 39).

[8] Peter Sjögren. "Operators associated with the Hermite semigroup—a survey". In: *J. Fourier Anal. Appl.* 3.Special Issue (1997), 813–823. DOI: 10.1007/BF02656487 (see p. 40).

[9] Elias M. Stein. *Harmonic analysis: real-variable methods, orthogonality, and oscillatory integrals*. Vol. 43. Princeton Mathematical Series. With the assistance of Timothy S. Murphy, Monographs in Harmonic Analysis, III. Princeton, NJ: Princeton University Press, 1993, xiv+695 (see p. 38).

[10] Jonas Teuwen. "A note on Gaussian maximal functions". In: *Indagationes Mathematicae* 26.1 (2015), 106–112. DOI: 10.1016/j.indag.2014.07.017 (see p. 37).

3. The integral kernels of derivatives of the Ornstein–Uhlenbeck semigroup

This paper presents a closed-form expression for the integral kernels associated with the derivatives of the Ornstein-Uhlenbeck semigroup e^{tL}. Our approach is to expand the Mehler kernel into Hermite polynomials and applying the powers L^N of the Ornstein-Uhlenbeck operator to it, where we exploit the fact that the Hermite polynomials are eigenfunctions for L. As an application we give an alternative proof of the kernel estimates by [12], making all relevant quantities explicit.

3.1. Introduction

Much effort [2, 3, 5–9, 11–14] has gone into developing the harmonic analysis of the *Ornstein-Uhlenbeck operator* (1.6) on the space $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$, where γ is the Gaussian measure (1.2). As was mentioned in Chapter 2 this operator can be viewed as the Gaussian counterpart of the Laplace operator Δ. Indeed, one has $L = -\nabla^*\nabla$, where ∇ is the the usual gradient and the ∇^* is its adjoint in $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$. It is a classical fact that the semigroup operators e^{tL}, $t > 0$, are integral operators of the form (1.30) Developing a Hardy space theory for L is the subject of active current research [7, 12]. In this theory the derivatives $(\mathrm{d}^k/\mathrm{d}t^k)\mathrm{e}^{tL} = L^N\mathrm{e}^{tL}$ play an important role. The aim of the present paper is to derive closed form expressions for the integral kernels of these derivatives, that is, to determine explicitly the kernels M_t^N such that we have the identity

$$L^N\mathrm{e}^{tL}u(\cdot) = \int_{\mathbf{R}^d} M_t^N(\cdot, y)u(y)\,\mathrm{d}\gamma(y). \tag{3.1}$$

Direct application of the derivatives $\mathrm{d}^N/\mathrm{d}t^N$ to the Mehler kernel yields expressions which become intractible even for small values of N. Our approach will be to expand the Mehler kernel in terms of the L^2-normalised Hermite polynomials and then to apply L^N to it, thus exploiting the fact that the Hermite polynomials are eigenfunctions for L.

As an application of our main result, which is proved in section 3.5 after developing some preliminary material in the sections 3.2-3.4, we shall give a direct proof for the kernel bounds of [12] in section 3.6.

3.2. Preliminaries

In this preliminary section we collect some standard properties of Hermite polynomials and their relationship with the Ornstein-Uhlenbeck operator. Most of this material is classical and can be found in [13, 15] and Chapter 1.

3.2.1. Hermite polynomials

The *Hermite polynomials* H_n, $n \geq 0$, are defined by Rodrigues's formula (1.11)

$$H_n(x) := (-1)^n e^{x^2} \partial_x^n e^{-x^2}.$$

Their L^2-normalizations (h_n, $n \geqslant 0$ given in (1.19) form an orthonormal basis for $L^2(\mathbf{R}, d\gamma)$. We shall use the fact that the generating function for the Hermite polynomials (1.14) is given by

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n = e^{2tx-t^2}.$$

The relationship with the Ornstein-Uhlenbeck operator is encoded in the eigenvalue identity $LH_n = -nH_n$, from which it follows that for all $t \geq 0$ we have $e^{tL}H_n = e^{-tn}H_n$. From this one quickly deduces that the Mehler kernel is given by

$$M_t(x,y) := \sum_{n=0}^{\infty} e^{-tn} h_n(x) h_n(y). \tag{3.2}$$

We will need two further identities for the Hermite polynomials which can be found, e.g., in [1, Chapter 18] and are derived in Chapter 1, the integral representation (1.12):

$$H_n(x) = \frac{(-2i)^n e^{x^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \xi^n e^{2ix\xi} e^{-\xi^2} \, d\xi$$

and the "binomial" identity (1.24):

$$H_n(x+y) = \sum_{k=0}^{n} \binom{n}{k} (2y)^{n-k} H_k(x).$$

3.2.2. Hermite polynomials in several variables

The Hermite polynomials on $\mathbf{R}^d$, introduced in Section 1.12, are defined, for multiindices $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbf{N}^d$ by the tensor extensions

$$H_\alpha(x) := \prod_{n=1}^{d} h_{\alpha_i}(x_i),$$

for $x = (x_1, \dots, x_d)$ in $\mathbf{R}^d$. The normalized Hermite polynomials

$$h_\alpha := \frac{H_\alpha}{\sqrt{2^{|\alpha|}\alpha!}}, \quad \text{where } \alpha! = \alpha_1! \cdot \dots \cdot \alpha_d! \tag{3.3}$$

form an orthonormal basis in $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$, and we have the eigenvalue identity

$$LH_\alpha = -|\alpha| H_\alpha, \quad \text{where } |\alpha| = \alpha_1 + \dots + \alpha_d.$$

If we consider the action of $L^N \mathrm{e}^{tL}$ on a Hermite polynomial h_α, through the multinomial theorem applied to $|\alpha|^k$ we get (writing L_d for the operator L in dimension d and L_1 for the operator L in dimension 1)

$$\begin{aligned} L_d^N \mathrm{e}^{tL} h_\alpha(x) &= |\alpha|^N \mathrm{e}^{-t|\alpha|} h_{\alpha_1}(x_1) \cdot \dots \cdot h_{\alpha_d}(x_d) \\ &= \sum_{|n|=N} \binom{N}{n_1, n_2, \dots, n_d} \prod_{i=1}^{n} \alpha_i^{n_i} \mathrm{e}^{-t\alpha_i} h_{\alpha_i}(x_i) \\ &= \sum_{|n|=N} \binom{N}{n_1, n_2, \dots, n_d} \prod_{i=1}^{n} L_1^{n_i} \mathrm{e}^{tL_1} h_{\alpha_i}(x_i). \end{aligned} \tag{3.4}$$

Using this, we can reduce the question of computing the d-dimensional integral Mehler kernel to the formula for the one-dimension Mehler kernel.

3.3. A combinatorial lemma

From now on we concentrate on the Ornstein-Uhlenbeck operator L in one dimension, i.e., in $L^2(\mathbf{R}, \mathrm{d}\gamma)$. We are going to follow the approach of [13]. Recalling the identity $Lh_n = -nh_n$, we will apply L^N to the generating function of the Hermite polynomials (1.14). A problem which immediately occurs is that Δ and $\langle x, \nabla \rangle$ do not commute, and because of this we cannot use a standard binomial formula to evaluate L^N. Instead, we note that

$$Lg = -t\partial_t g.$$

In particular this implies that

$$L^N g = (-1)^k D_N g,$$

where

$$D_N := \underbrace{t\partial_t \circ t\partial_t \circ \cdots \circ t\partial_t}_{k \text{ times}} = (t\partial_t)^N.$$

The following lemma will be very useful.

3.1 Lemma We have

$$D_N = \sum_{n=0}^{N} \left\{ {N \atop n} \right\} t^n \partial_t^n, \tag{3.5}$$

where $\left\{ {N \atop n} \right\}$ are the Stirling numbers of the second kind.

The Stirling numbers of the second kind are quite well-known combinatorial objects. For the sake of completeness we will state their definition and recall some relevant properties below. For more information we refer the reader to [4]. The related Stirling numbers of the first kind will not be needed here.

We begin by recalling the definition of *falling factorial*

$$(j)_n := j(j-1)\dots(j-n+1) = \frac{j!}{(j-n)!}, \tag{3.6}$$

for non-negative integers $k \geqslant n$.

3.2 Definition For non-negative integers $N \geq n$, the number *Stirling number of the second kind* $\left\{ N \atop n \right\}$ is defined as the number of partitions of an N-set into n non-empty subsets.

These numbers satisfy the recursion identity

$$\left\{ N \atop n \right\} = N \left\{ N-1 \atop n \right\} + \left\{ N-1 \atop n-1 \right\}.$$

For all non-negative integers j and k one has the generating function identity

$$j^N = \sum_{n=0}^{N} \left\{ N \atop n \right\} (j)_n. \tag{3.7}$$

3.4. Weyl Polynomials

Before turning to the proof of lemma 3.1, let us already mention that it only depends on the commutator identity $[t, \partial_t] = -1$. This brings us to the observation that *Weyl polynomials* provide the natural habitat for our expressions. Rougly speaking, a Weyl polynomial is a polynomial in two non-commuting variables x and y which satisfy the commutator identity $[x, y] = -1$. This is made more precise in the following definition.

3.3 Definition The *Weyl algebra* over a field $\mathscr{F}$ of characteristic zero is the ring $\mathscr{F}\langle x, y\rangle$ of all polynomials of the form $p(x,y) = \sum_{m=0}^{M}\sum_{n=0}^{N} c_{m,n}x^m y^n$ with coefficients $c_{mn} \in \mathscr{F}$ in two noncommuting variables x and y which satisfy the commutator identity

$$[x,y] := xy - yx = -1.$$

We now have the following abstract version of lemma 3.1:

3.4 Lemma In the Weyl algebra $\mathscr{F}\langle x, y\rangle$ we have the identity

$$(xy)^m = \sum_{i=1}^{m} \left\{ {m \atop i} \right\} x^i y^i,$$

where $\left\{ {m \atop i} \right\}$ are the Stirling numbers of the second kind.

As a preparation for the proof of lemma 3.4 we make a couple of easy computations. If we set $D := xy$, then

$$\begin{aligned} Dx^m &= x^m D + m x^m, \\ Dy^m &= y^m D - m y^m. \end{aligned} \tag{3.8}$$

This can be shown by induction on m. For instance, note that

$$Dx^m = x(D+1)x^{m-1} = xDx^{m-1} + x^m.$$

If we take this a bit further and have $p \in \mathscr{F}[D]$, then

$$p(D)x^m = x^m p(D+m), \tag{3.9}$$

$$p(D)y^m = y^m p(D-m). \tag{3.10}$$

The m-th powers, $m \geq 1$, of x and y satisfy

$$x^m y^m = \prod_{i=0}^{m-1}(D-i), \tag{3.11}$$
$$y^m x^m = \prod_{i=1}^{m}(D+i).$$

This can be seen using induction:

$$x^{m+1}y^{m+1} = x^m D y^m \overset{(3.10)}{=} x^m y^m (D-m)$$

and

$$y^{m+1}x^{m+1} = y^m(D+1)x^m = y^m D x^m + y^m x^m \overset{(3.9)}{=} y^m x^m (D+(m+1)).$$

3.5 Definition The *weighted degree* of a monomial $x^m y^n \in \mathscr{F}\langle x, y\rangle$ is the integer $m-n$. A polynomial in $\mathscr{F}\langle x, y\rangle$ is said to be *homogeneous of weighted degree* j if all its constituting monomials have weighted degree j.

Left multiplication by xy is *homogeneity preserving*, i.e., for all $j \in \mathbf{Z}$ it maps the set of homogeneous monomials of weighted degree j into itself. To prove this, first consider a monomial $x^m y^n$ of weighted degree $j = m-n$. Then,

$$\begin{aligned}(xy)x^m y^n &\overset{(3.8)}{=} (x^m(xy) + mx^m)y^n \\ &= x^m(xy)y^n + mx^m y^n \\ &= x^{m+1}y^{n+1} + mx^m y^n,\end{aligned}$$

and we see that weighted degree of homogeneity is indeed preserved. The general case follows immediately. Through (3.11) we conclude that left multiplication $x^k y^k$ is homogeneity preserving as well, for all non-negative integers k. We claim that left multiplication by $x^i y^j$ is homogeneity preserving only if $i = j$. To see this note that

$$yx^i y^j = x^i y^{i+j} + ix^{i-1} y^j$$

from which we can deduce that

$$x^m y^M x^n y^N = x^{n+m} y^{N+M} + \text{ lower order terms.}$$

From which the claim follows.

Finally, a polynomial is homogeneity preserving if and only if all of its constituting monomials have this property. If this were not to be the case we could look at the highest-order non-homogeneous term and note from above $x^m y^M x^n y^N$ would give terms of a lower order in the polynomial expansion which cannot cancel as they have different powers of x or y.

It follows from these observations that

$$F_0 := \left\{ \sum_{n=0}^{N} c_n x^n y^n \;\middle|\; N \in \mathbf{N},\, c_1, \ldots, c_N \in \mathscr{F} \right\}$$

is precisely the set of *homogeneity preserving polynomials* in $\mathscr{F}\langle x, y\rangle$.

Now everything is in place to give the proof of lemma 3.4.

Proof of lemma 3.4. As $(xy)^k$ is homogeneity preserving, we infer that there are coefficients a_i^k in $\mathscr{F}$ such that

$$(xy)^k = \sum_{i=0}^{k} a_i^k x^i y^i. \tag{3.12}$$

We will apply x^j to the right on both sides of (3.12) and derive an expression for the a_i^k. First note that (3.9) gives

$$(xy)^k x^j = x^j (xy + j)^k,$$

and (3.11) together with (3.9) gives

$$x^i y^i x^j \overset{(3.11)}{=} \prod_{\ell=0}^{i-1}(xy-\ell)x^j \overset{(3.9)}{=} x^j \prod_{\ell=0}^{i-1}(xy-\ell+j).$$

Hence, to find the coefficients a_i^k it is sufficient to consider

$$(xy+j)^k = \sum_{i=0}^{k} a_n^k \prod_{\ell=0}^{i-1}(xy-\ell+j).$$

Comparing the constant terms on both the left-hand side and right-hand side, we find

$$j^k = \sum_{i=0}^{k} a_i^k \prod_{\ell=0}^{i-1}(j-\ell) = \sum_{i=0}^{k} a_i^k (j)_i, \tag{3.13}$$

where $(j)_i$ is the falling factorial as in (3.6). Comparing (3.13) with the generating function of the Stirling numbers of the second kind $\left\{ {k \atop i} \right\}$ as given in (3.7), we see that $a_i^k = \left\{ {k \atop i} \right\}$. This concludes the proof of lemma 3.4. ■

3.5. The integral kernel of $L^N e^{tL}$

As mentioned before, as a first step we would like to apply D_N to the generating function $g(x,t) := e^{-2tx+t^2} = e^{-(x-t)^2+x^2}$ for the Hermite polynomials (1.14). We first compute the action of ∂_t^N on the generating function.

3.6 Lemma We have

$$\partial_t^N e^{-(x-t)^2+x^2} = e^{-(x-t)^2+x^2} H_N(x-t).$$

Proof. We first note that,

$$\partial_t e^{-(x-t)^2} = 2(x-t)e^{-(x-t)^2} = -\partial_x e^{-(x-t)^2}.$$

Using this we get

$$\begin{aligned}\partial_t^N \mathrm{e}^{-(x-t)^2+x^2} &= \mathrm{e}^{x^2}\partial_t^N \mathrm{e}^{-(x-t)^2}\\ &= \mathrm{e}^{x^2}\partial_t^{N-1}\partial_t \mathrm{e}^{-(x-t)^2}\\ &= -\mathrm{e}^{x^2}\partial_t^{N-1}\partial_x \mathrm{e}^{-(x-t)^2}\\ &= (-1)^2\mathrm{e}^{x^2}\partial_t^{N-2}\partial_x^2 \mathrm{e}^{-(x-t)^2}.\end{aligned}$$

If we iterate this further we obtain for all natural numbers N that

$$\partial_t^N \mathrm{e}^{-(x-t)^2+x^2} = (-1)^N \mathrm{e}^{x^2}\partial_x^N \mathrm{e}^{-(x-t)^2}.$$

By a change of variables,

$$\partial_t^N \mathrm{e}^{-(x-t)^2+x^2} = (-1)^N \mathrm{e}^{-(x-t)^2+x^2}\mathrm{e}^{(x-t)^2}\partial_y^N \mathrm{e}^{-y^2}\Big|_{y=x-t}.$$

Hence, by (1.11),

$$\partial_t^N \mathrm{e}^{-(x-t)^2+x^2} = \mathrm{e}^{-(x-t)^2+x^2}H_N(x-t). \qquad \blacksquare$$

3.7 Lemma For all $x \in \mathbf{R}$ and $t > 0$ we have

$$L^N \mathrm{e}^{-(x-t)^2+x^2} = (-1)^N \mathrm{e}^{-(x-t)^2+x^2}\sum_{n=0}^{N}\left\{ {N \atop n} \right\} t^n H_n(x-t). \tag{3.14}$$

Proof. This is now easy to prove. Recalling that $Lg = -t\partial_t g$ and using (3.5), we get

$$\begin{aligned}L^N \mathrm{e}^{-(x-t)^2+x^2} &= D_N \mathrm{e}^{-(x-t)^2+x^2}\\ &= (-1)^N \sum_{n=0}^{N}\left\{ {N \atop n} \right\} t^n \partial_t^n \mathrm{e}^{-(x-t)^2+x^2}\\ &= (-1)^N \mathrm{e}^{-(x-t)^2+x^2}\sum_{n=0}^{N}\left\{ {N \atop n} \right\} t^n H_n(x-t).\end{aligned} \qquad \blacksquare$$

Our next theorem is the main result of this paper and provides an explicit expression for the integral kernel of $L^N e^{tL}$.

3.8 Theorem Let L be the Ornstein-Uhlenbeck operator on $L^2(\mathbf{R}^d, \mathrm{d}\gamma)$, let $t > 0$, and let $N \geq 0$ be an integer. The integral kernel M_t^N of $L^N \mathrm{e}^{tL}$ is given by

$$M_t^N(x,y) = M_t(x,y) \sum_{|n|=N} \binom{N}{n_1,\dots,n_d} \prod_{i=1}^{d} \sum_{m_i=0}^{n_i} \sum_{\ell_i=0}^{m_i} 2^{-m_i} \left\{ {n_i \atop m_i} \right\} \binom{m_i}{\ell_i} \\ \times \left(-\frac{\mathrm{e}^{-t}}{\sqrt{1-\mathrm{e}^{-2t}}} \right)^{2m_i-\ell_i} H_{\ell_i}(x_i) H_{2m_i-\ell_i}\left(\frac{x_i \mathrm{e}^{-t} - y_i}{\sqrt{1-\mathrm{e}^{-2t}}} \right).$$

Proof. We first prove the result for $d = 1$. Pulling L^N through the integral expression (3.1) for e^{tL} involving the Mehler kernel, we must find a suitable expression for the kernel $M_t^N(\cdot, y) = L^N M_t(\cdot, y)$. Using (3.2) and the normalization of H_m in (3.3) we get

$$\begin{aligned} M_t^N(x,y) &= L^N \sum_{m=0}^{\infty} \frac{\mathrm{e}^{-tm}}{m!} \frac{1}{2^m} H_m(x) H_m(y) \\ &\overset{(1.12)}{=} L^N \sum_{m=0}^{\infty} \frac{\mathrm{e}^{-tm}}{m!} \frac{1}{2^m} H_m(x) \frac{(-2i)^m}{\sqrt{\pi}} \mathrm{e}^{y^2} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} \xi^m \mathrm{e}^{2iy\xi} \,\mathrm{d}\xi \\ &= L^N \frac{\mathrm{e}^{y^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} \mathrm{e}^{2iy\xi} \sum_{m=0}^{\infty} \frac{1}{m!} H_m(x) (-i\xi \mathrm{e}^{-t})^m \,\mathrm{d}\xi \\ &\overset{(1.14)}{=} L^N \frac{\mathrm{e}^{y^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} \mathrm{e}^{2iy\xi} \mathrm{e}^{-(x+i\xi \mathrm{e}^{-t})^2 + x^2} \,\mathrm{d}\xi. \end{aligned}$$

The operator L^N is applied with respect to x here, so by lemma 3.7 we get

$$\begin{aligned}
M_t^N(x,y) &= \frac{\mathrm{e}^{y^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{-\xi^2} \mathrm{e}^{2iy\xi} L^N \mathrm{e}^{-(x+i\xi\mathrm{e}^{-t})^2+x^2}\,\mathrm{d}\xi \\
&\overset{(3.14)}{=} (-1)^N \frac{\mathrm{e}^{x^2+y^2}}{\sqrt{\pi}} \sum_{m=0}^{N} \left\{ {N \atop m} \right\} \\
&\quad \times \int_{-\infty}^{\infty} \mathrm{e}^{2iy\xi} \mathrm{e}^{-(x+i\xi\mathrm{e}^{-t})^2} (i\xi\mathrm{e}^{-t})^m H_m(y+i\xi\mathrm{e}^{-t}) \mathrm{e}^{-\xi^2}\,\mathrm{d}\xi,
\end{aligned}$$

where in last line we have used the analytic continuation of the algebraic identity (3.14). Similarly we can expand $H_m(y+i\xi\mathrm{e}^{-t})$ using (1.24). This gives

$$H_m(y+i\xi\mathrm{e}^{-t}) = \sum_{\ell=0}^{m} \binom{m}{\ell} H_\ell(y)(2i\xi\mathrm{e}^{-t})^{m-\ell},$$

so that M_t^N can be written as

$$\begin{aligned}
M_t^N = (-1)^N \frac{\mathrm{e}^{x^2+y^2}}{\sqrt{\pi}} \sum_{m=0}^{N} \sum_{\ell=0}^{m} \left\{ {N \atop m} \right\} \binom{m}{\ell} H_\ell(y) 2^{m-\ell} \\
\times \int_{-\infty}^{\infty} \mathrm{e}^{2iy\xi-\xi^2} \mathrm{e}^{-(x+i\xi\mathrm{e}^{-t})^2} (i\xi\mathrm{e}^{-t})^{2m-\ell}\,\mathrm{d}\xi.
\end{aligned}$$

If we set $M = 2m-\ell$, this reduces our task to computing the integral

$$\begin{aligned}
&\frac{\mathrm{e}^{x^2+y^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{2iy\xi-\xi^2} \mathrm{e}^{-(x+i\xi\mathrm{e}^{-t})^2} (i\xi\mathrm{e}^{-t})^M\,\mathrm{d}\xi \\
&\qquad = \frac{\mathrm{e}^{y^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{e}^{2i(x\mathrm{e}^{-t}-y)\xi} \mathrm{e}^{-(1-\mathrm{e}^{-2t})\xi^2} (i\xi\mathrm{e}^{-t})^M\,\mathrm{d}\xi. \quad (3.15)
\end{aligned}$$

To make the computation less convolved, let us set

$$\alpha_t := \sqrt{1-\mathrm{e}^{-2t}}, \text{ and, } \beta_t(x,y) := \frac{x\mathrm{e}^{-t}-y}{\sqrt{1-\mathrm{e}^{-2t}}}.$$

This allows us to write the exponential in the integral (3.15) as

$$\mathrm{e}^{2i(x\mathrm{e}^{-t}-y)\xi}\mathrm{e}^{-(1-\mathrm{e}^{-2t})\xi^2} = \mathrm{e}^{2i\alpha_t\beta_t(x,y)\xi}\mathrm{e}^{-\alpha_t^2\xi^2}.$$

This reduces the problem, after the substitution $\alpha_t\xi \to \xi$, to computing the integral

$$\frac{\mathrm{e}^{y^2}}{\sqrt{\pi}}\frac{i^M\mathrm{e}^{-Mt}}{\alpha_t^{M+1}}\int_{-\infty}^{\infty}\mathrm{e}^{2i\beta_t(x,y)\xi}\mathrm{e}^{-\xi^2}\xi^M\,\mathrm{d}\xi.$$

The final integral is an integral expression for the Hermite polynomials (1.12), so

$$\begin{aligned}\frac{\mathrm{e}^{y^2}}{\sqrt{\pi}}\frac{i^M\mathrm{e}^{-Mt}}{\alpha_t^{M+1}}&\int_{-\infty}^{\infty}\mathrm{e}^{2i\beta_t(x,y)\xi}\mathrm{e}^{-\xi^2}\xi^M\,\mathrm{d}\xi\\ &\stackrel{(1.12)}{=}\mathrm{e}^{y^2-\beta_t(x,y)^2}\frac{1}{\alpha_t^{M+1}}\frac{(-1)^M\mathrm{e}^{-Mt}}{2^M}H_M(\beta_t(x,y)).\end{aligned}$$

Next we note that $\exp(y^2-\beta_t(x,y)^2)\alpha_t^{-1} = M_t$, the Mehler kernel from (1.30). Hence,

$$\begin{aligned}M_t^N(x,y) = M_t(x,y)\sum_{m=0}^{N}\sum_{\ell=0}^{m}\binom{m}{\ell}\left\{{N \atop m}\right\}\left(-\frac{\mathrm{e}^{-t}}{\sqrt{1-\mathrm{e}^{-2t}}}\right)^{2m-\ell}2^{-m}\\ \times H_\ell(x)H_{2m-\ell}\left(\frac{x\mathrm{e}^{-t}-y}{\sqrt{1-\mathrm{e}^{-2t}}}\right).\end{aligned}$$

Applying (3.4) we get the result in d dimensions. ■

3.6. An application

As an application of our main result, in this section we give an alternative proof of the bounds on the kernels K and $\tilde{K}$ of [12] (see the definition below), making the dependence on the parameters more explicit. These kernels play a central role in the study of the Hardy space $H^1(\mathbf{R}^d, \mathrm{d}\gamma)$ in [12], where the standard Calderón reproducing formula is replaced by

$$u = C\int_0^\infty (t^2L)^{N+1}\mathrm{e}^{\frac{t^2}{\alpha}L}u\frac{\mathrm{d}t}{t} + \int_{\mathbf{R}^d} u\,\mathrm{d}\gamma,$$

where C is a suitable constant only depending on N and α (this can be seen by letting u be a Hermite polynomial). The kernels K and $\tilde{K}$ then occur in several decompositions, and the estimates below allow them to be related to classical results about the Mehler kernel.

3.9 Definition We define the kernels K and $\tilde{K}$ by

$$\int_{\mathbf{R}^d} K_{t^2,N,\alpha}(x,y)u(y)\,\mathrm{d}\gamma(y) = (t^2L)^N\mathrm{e}^{\frac{t^2}{\alpha}L}u(x),$$
$$\int_{\mathbf{R}^d} \tilde{K}_{t^2,N,\alpha,j}(x,y)u(y)\,\mathrm{d}\gamma(y) = (t^2L)^N\mathrm{e}^{\frac{t^2}{\alpha}L}t\partial_{x_j}^*u(x).$$

Note that the operators on the right-hand sides are indeed given by integral kernels: the first is a scaled version of the operator we have already been studying, and a duality argument implies that the second is given by the integral kernel

$$\tilde{K}_{t^2,N,\alpha,j}(x,y) = t\partial_{x_j}K_{t^2,N,\alpha}(x,y).$$

Thus, both kernels are given as appropriate derivatives of the Mehler kernel.

We begin with a technical lemma which is a rephrased version of [12, Lemma 3.4]. One should take note that we define the kernels with respect to the Gaussian measure whereas, [12] defines these with respect to the Lebesgue measure.

3.10 Lemma For all $\alpha > 1$ and all $t > 0$ and x, y in $\mathbf{R}^d$ we have

$$\frac{|\mathrm{e}^{-\frac{t}{\alpha}}x - y|^2}{1 - e^{-2\frac{t}{\alpha}}} \geqslant \frac{\alpha}{2}\mathrm{e}^{-2t}\frac{|\mathrm{e}^{-t}x - y|^2}{1 - \mathrm{e}^{-2t}} - \frac{t^2 \min(|x|^2, |y|^2)}{1 - \mathrm{e}^{-2\frac{t}{\alpha}}}.$$

Additionally, we have

$$\alpha \mathrm{e}^{-2t} \leqslant \frac{1 - \mathrm{e}^{-2t}}{1 - \mathrm{e}^{-2\frac{t}{\alpha}}} \leqslant \alpha. \tag{3.16}$$

3.11 Theorem Let N be a positive integer, $0 < t < T$. The for all large enough $\alpha > 1$ we have

1. If $t|x| \leqslant C$, then

$$|K_{t^2,\alpha,N}(x,y)| \lesssim_{T,N} c_\alpha M_{t^2}(x,y) \exp\left(-\frac{\alpha}{8\mathrm{e}^{2T}} \frac{|\mathrm{e}^{-t^2}x - y|^2}{1 - \mathrm{e}^{-2t^2}}\right).$$

2. If $t|x| \leqslant C$, then

$$|\tilde{K}_{t^2,\alpha,N,j}(x,y)| \lesssim_{T,N} c_\alpha M_{t^2}(x,y) \exp\left(-\frac{\alpha}{8\mathrm{e}^{2T}} \frac{|\mathrm{e}^{-t^2}x - y|^2}{1 - \mathrm{e}^{-2t^2}}\right),$$

where $c_\alpha := \alpha \exp\left(\frac{\alpha}{2}C^2\right)$.

Proof. For $K_{t^2,\alpha,N}$, we use Theorem 3.8 to obtain, after taking absolute values,

$$\begin{aligned}
&|K_{t^2,\alpha,N}(x,y)| \\
&\quad \leqslant M_{\frac{t^2}{\alpha}}(x,y) \sum_{|k|=N} \binom{N}{n_1,\dots,n_d} \prod_{i=1}^{d} t^{2k_i} \sum_{\ell_i=0}^{n_i} \sum_{m_i=0}^{m_i} 2^{-m_i} \binom{m_i}{\ell_i} \left\{ {n_i \atop m_i} \right\} \\
&\qquad \times \left(\frac{\mathrm{e}^{-\frac{t^2}{\alpha}}}{\sqrt{1 - \mathrm{e}^{-2\frac{t^2}{\alpha}}}} \right)^{2m_i - \ell_i} |H_{\ell_i}(x_i)| \left| H_{2m_i - \ell_i}\left(\frac{x_i \mathrm{e}^{-\frac{t^2}{\alpha}} - y_i}{\sqrt{1 - \mathrm{e}^{-2\frac{t^2}{\alpha}}}} \right) \right|.
\end{aligned}$$

Recalling that $\ell_1 + \cdots + \ell_d \leqslant N$, using the assumptions $t \leqslant T$ and $t|x| \leqslant C$ we can bound $t^{2k_i}|H_{\ell_i}(x)|$ by considering the highest order term to obtain

$$t^{2k_i}|H_{\ell_i}(x)| \lesssim_{C,N,T} 1.$$

Using (3.16) we proceed by looking at

$$\begin{aligned}
M_{\frac{t^2}{\alpha}}(x,y) = M_{t^2}(x,y)&\left(\frac{1-\mathrm{e}^{-2t^2}}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right)^{1/2} \\
&\times \exp\left(\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\right)\exp\left(-\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x-y|^2}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right) \\
&\leq \alpha M_{t^2}(x,y)\exp\left(\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\right)\left[\exp\left(-\frac{1}{2}\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x-y|^2}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right)\right]^2.
\end{aligned}$$

We can now bound the final Hermite polynomial in the expression of the kernel. Setting $M_i = 2m_i - \ell_i$ we get

$$\begin{aligned}
&\left(\frac{\mathrm{e}^{-\frac{t^2}{\alpha}}}{\sqrt{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}}\right)^{M_i}\left|H_{M_i}\left(\frac{\mathrm{e}^{-\frac{t^2}{\alpha}}x_i-y_i}{\sqrt{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}}\right)\right| \\
&\qquad\lesssim_N \left(\frac{\mathrm{e}^{-\frac{t^2}{\alpha}}}{\sqrt{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}}\right)^{M_i}\left(\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x_i-y_i|}{\sqrt{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}}\right)^{M_i} \leq \left(\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x_i-y_i|}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right)^{M_i}.
\end{aligned}$$

Also,

$$\left(\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x_i-y_i|}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right)^{M_i}\exp\left(-\frac{1}{2}\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x_i-y_i|^2}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\right) \lesssim 1.$$

Putting these estimates together, using Lemma 3.10, and taking $\alpha > 1$ so large that

$$1-\frac{\alpha}{4\mathrm{e}^{2T}} \leq -\frac{\alpha}{8\mathrm{e}^{2T}} \quad \text{and} \quad 1-\mathrm{e}^{-2\frac{t^2}{\alpha}} \geq \frac{t^2}{\alpha},$$

we obtain

$$
\begin{aligned}
|K_{t^2,\alpha,N}(x,y)| &\lesssim_{T,N} \alpha M_{t^2}(x,y)\exp\Big(\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\Big)\exp\Big(-\frac{1}{2}\frac{|\mathrm{e}^{-\frac{t^2}{\alpha}}x-y|^2}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\Big)\\
&\leqslant \alpha M_{t^2}(x,y)\exp\Big(\Big(1-\frac{\alpha}{4\mathrm{e}^{2T}}\Big)\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\Big)\\
&\qquad\times\exp\Big(\frac{1}{2}\frac{t^4|x|^2}{1-\mathrm{e}^{-2\frac{t^2}{\alpha}}}\Big)\\
&\leqslant \alpha M_{t^2}(x,y)\exp\Big(-\frac{\alpha}{8\mathrm{e}^{2T}}\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\Big)\exp\Big(\frac{\alpha}{2}t^2|x|^2\Big)\\
&\leqslant \alpha\exp\Big(\frac{\alpha}{2}C^2\Big)M_{t^2}(x,y)\exp\Big(-\frac{\alpha}{8\mathrm{e}^{2T}}\frac{|\mathrm{e}^{-t^2}x-y|^2}{1-\mathrm{e}^{-2t^2}}\Big),
\end{aligned}
$$

using $t|x|\leqslant C$ in the final step.

For the bound on $\tilde{K}$ we consider

$$
\begin{aligned}
t\partial_{x_i}\Big[H_{\ell_i}(x_i)H_{m_i}\Big(\frac{x_i\mathrm{e}^{-t}-y_i}{\sqrt{1-\mathrm{e}^{-2t}}}\Big)\Big] &= tH_{m_i}\Big(\frac{x_i\mathrm{e}^{-t}-y_i}{\sqrt{1-\mathrm{e}^{-2t}}}\Big)\partial_{x_i}H_\ell(x_i)\\
&\quad + H_{\ell_i}(x_i)t\partial_{x_i}H_{m_i}\Big(\frac{x_i\mathrm{e}^{-t}-y_i}{\sqrt{1-\mathrm{e}^{-2t}}}\Big).
\end{aligned}
$$

So, as the first term on the right-hand side just decreases in degree we look at

$$
t\partial_{x_i}\Big(\frac{x_i\mathrm{e}^{-t}-y_i}{\sqrt{1-\mathrm{e}^{-2t}}}\Big)^{m_i} = m_i\Big(\frac{x_i\mathrm{e}^{-t}-y_i}{\sqrt{1-\mathrm{e}^{-2t}}}\Big)^{m_i-1}t\frac{\mathrm{e}^{-t}}{\sqrt{1-\mathrm{e}^{-2t}}}.
$$

The last term is bounded as $t\downarrow 0$, and the rest of the proof is as before. ∎

3.7. Acknowledgments

This work was partially supported by NWO-VICI grant 639.033.604 of the Netherlands Organisation for Scientific Research (NWO).

The author wishes to thank Alex Amenta and Mikko Kemppainen for inspiring discussions.

References

[1] *NIST Digital Library of Mathematical Functions*. http://dlmf.nist.gov/, Release 1.0.10 of 2015-08-07. Online companion to [10] (see pp. 51, 68).

[2] E. Harboure, J.L. Torrea, and B. Viviani. "On the search for weighted inequalities for operators related to the Ornstein-Uhlenbeck semigroup". In: *Mathematische Annalen* 318.2 (Oct. 2000), 341–353. DOI: 10.1007/PL00004424 (see p. 50).

[3] Mikko Kemppainen. "An L^1-estimate for certain spectral multipliers associated with the Ornstein–Uhlenbeck operator". In: (2015). eprint: arXiv:1508.06102 (see p. 50).

[4] J. H. van Lint and R. M. Wilson. *A course in combinatorics*. Second. Cambridge University Press, Cambridge, 2001, xiv+602. DOI: 10.1017/CBO9780511987045 (see p. 54).

[5] Jan Maas, Jan van Neerven, and Pierre Portal. "Whitney coverings and the tent spaces $T^{1,q}(\gamma)$ for the Gaussian measure". In: *Arkiv för Matematik* 50.2 (Apr. 2011), 379–395. DOI: 10.1007/s11512-010-0143-z (see p. 50).

[6] Jan Maas, Jan Van Neerven, and Pierre Portal. "Conical square functions and non-tangential maximal functions with respect to the gaussian measure". In: *Publicacions Matematiques* 55.2 (Mar. 2011), 313–341. DOI: 10.5565/PUBLMAT_55211_03. arXiv: 1003.4092 (see p. 50).

[7] Giancarlo Mauceri and Stefano Meda. "BMO and H^1 for the Ornstein–Uhlenbeck operator". In: *Journal of Functional Analysis* 252.1 (Nov. 2007), 278–313. DOI: 10.1016/j.jfa.2007.06.017 (see p. 50).

[8] Giancarlo Mauceri, Stefano Meda, and Peter Sjögren. "Endpoint estimates for first-order Riesz transforms associated to the Ornstein–Uhlenbeck operator". In: *Rev. Mat. Iberoam.* 28.1 (2012), 77–91. DOI: 10.4171/RMI/667 (see p. 50).

[9] Benjamin Muckenhoupt. "Hermite conjugate expansions". In: *Trans. Amer. Math. Soc.* 139 (1969), 243–260 (see p. 50).

[10] F. W. J. Olver et al., eds. *NIST Handbook of Mathematical Functions*. Print companion to [1]. New York, NY: Cambridge University Press, 2010 (see p. 67).

[11] Ebner Pineda and Wilfredo Urbina R. "Non tangential convergence for the Ornstein-Uhlenbeck semigroup". In: *Divulgaciones Matematicas* 16.2 (2008), 107–124. arXiv: `0611040 [math]` (see p. 50).

[12] Pierre Portal. "Maximal and quadratic gaussian Hardy spaces". In: *Revista Matematica Iberoamericana* 30 (Mar. 2014), 79–108. DOI: `10.4171/rmi/770`. arXiv: `1203.1998` (see pp. 49, 50, 62, 63).

[13] Peter Sjögren. "Operators associated with the Hermite semigroup—a survey". In: *J. Fourier Anal. Appl.* 3.Special Issue (1997), 813–823. DOI: `10.1007/BF02656487` (see pp. 50, 51, 53).

[14] Jonas Teuwen. "A note on Gaussian maximal functions". In: *Indagationes Mathematicae* 26.1 (2015), 106–112. DOI: `10.1016/j.indag.2014.07.017` (see p. 50).

[15] Sundaram Thangavelu. *Lectures on Hermite and Laguerre expansions*. Mathematical Notes. With a preface by Robert S. Strichartz. Princeton University Press, Princeton, NJ, 1993, xviii+195 (see p. 51).

4. Failure of the L^1–L^p off-diagonal estimates for the Ornstein–Uhlenbeck semigroup and $p > 1$

In the development of Gaussian harmonic analysis one would in the ideal case have the same tools at one's disposal as in the Euclidean case. This chapter shows that off-diagonal estimates cannot exist for the Ornstein–Uhlenbeck operator with respect to the Gaussian measure.

This chapter is joint work with Alex Amenta.

4.1. Introduction

The notion of off-diagonal estimates (also called off-diagonal bounds) has proven to be useful in the harmonic analysis of differential operators which lie beyond the scope of Calderón–Zygmund theory. Such estimates hold for the Laplacian on a Riemannian manifold (the so-called Davies–Gaffney estimates [2]), and for divergence-form elliptic operators $\operatorname{div} A\nabla$ with rough coefficients A on $\mathbf{R}^d$. They are especially useful in the analysis of operators whose heat semigroups do not have a smooth enough kernel.

In contrast to classical harmonic analysis where we have the heat semigroup in Gaussian harmonic analysis we are interested in the semigroup $(\mathrm{e}^{tL})_{t>0}$ associated with the Ornstein–Uhlenbeck operator (1.6) which is symmetric with respect to the Gaussian measure (1.2) on the Euclidean space $\mathbf{R}^d$.

As is well known[1], the Ornstein–Uhlenbeck semigroup $(\mathrm{e}^{tL})_{t>0}$ has an explicit kernel, called the Mehler kernel (1.33). Even though the Ornstein–Uhlenbeck semigroup has this kernel, it would still be useful to show that it satisfies some form of off-diagonal estimates; this would allow for generalisation to operators related to the Ornstein–Uhlenbeck operator by some kind of perturbation.

In the setting of a doubling metric measure space (X, d, μ), Auscher and Martell [1, Definition 3.1] define the following notion of *full L^p–L^q off-diagonal estimates*.

[1] see for instance the review of Sjögren [6], the introduction of [7] and the exposition in Section 1.3.4.

4.1 Definition Let $(\mathscr{X}, d, \mu)$ a doubling metric measure space. Let $1 \leqslant p \leqslant q \leqslant \infty$. We say that a family $\{T_t\}_{t>0}$ of sublinear operator satisfies $L^p(\mu)$–$L^q(\mu)$ full off-diagonal estimates if for some $\theta \geqslant 0$, with $\theta \neq 0$ when $p < q$, for all closed sets E and F, all f and all $t > 0$ we have that

$$\Big(\int_F |T_t \mathbf{1}_E f|^q \,\mathrm{d}\mu\Big)^{1/q} \lesssim t^{-\theta} \exp\Big(-c\frac{d^2(E,F)}{t}\Big)\Big(\int_E |f|^p \,\mathrm{d}\mu\Big)^{1/p}. \tag{4.1}$$

Since the Gaussian measure γ is non-doubling, this notion does not apply in the Gaussian setting. However, Mauceri and Meda [3] observed that γ is doubling when restricted to *admissible balls*, in the sense that $\gamma(B(x,2r)) \lesssim \gamma(B(x,r))$ when $r < \min(1, |x|^{-1})$. Therefore it is reasonable to expect that some adapted version of the Auscher–Martell definition of L^p–L^q off-diagonal estimates on balls holds for the Ornstein–Uhlenbeck operator, if we take admissibility in the sense of Mauceri–Meda into account. The purpose of this chapter is to demonstrate that such estimates fail.

While L^p–L^q estimates in general fail, the Ornstein–Uhlenbeck semigroup does satisfy L^2–L^2 off-diagonal estimates (similar to Davies–Gaffney estimates). These are of the following form which is due to A. McIntosh (unpublished manuscript) and is reproduced in [5, Example 6.1].

4.2 Theorem (McIntosh) Consider $u \in L^2(\mathbf{R}^d, \gamma)$ and let E, F be closed subsets of $\mathbf{R}^d$. Then we have

$$\Big(\int_F |\mathrm{e}^{tL}\mathbf{1}_E u|^2 \,\mathrm{d}\gamma\Big)^{1/2} \lesssim \frac{t}{d(E,F)} \exp\Big(-\frac{d(E,F)^2}{2t}\Big)\Big(\int_E |u|^2 \,\mathrm{d}\gamma\Big)^{1/2}.$$

Ideally we would like to improve this to some form of L^p–L^2 off-diagonal estimates for some $p < 2$.

It was shown by Nelson [4] that e^{tL} maps $L^p(\mathbf{R}^d, \gamma)$ boundedly into

$L^2(\mathbf{R}^d, \gamma)$ when $t > \sqrt{\log(p-1)}$.[2] This is in contrast to the situation for the ordinary heat semigroup $e^{t\Delta}$ on $\mathbf{R}^d$, which maps $L^p(\mathbf{R}^d)$ into $L^q(\mathbf{R}^d)$ for all $p \leqslant q$. However, this global result does not rule out the possibility of L^p–L^2 off-diagonal estimates.

In Section 4.3 we show that for all $p > 1$ the Ornstein–Uhlenbeck operator does not satisfy Auscher–Martell L^1–L^p full off-diagonal estimates.

Our results do not rule out the possibility of L^p–L^2 off-diagonal estimates for $p \in (1,2)$ for sufficiently large t depending on p. As the off-diagonal estimates can be heuristically seen as a tradeoff between diffusion and hypercontractivity, we can additionally prove that with $t_p := \sqrt{\log(p'-1)}$, $(e^{tL})_{t>t_p}$ satisfies $L^q - L^2$ off-diagonal estimates in some sense for all $q \in (p,2]$. Such a result would require more refined techniques than our naïve Mehler kernel lower bounds.

4.2. Motivation

Before we proceed we give an application where such estimates would naturally arise. Consider the operator π,

$$\pi u = \int_{m(\cdot)}^{\infty} (t^2 L)^{N+1} e^{t^2 L} u \frac{dt}{t}$$

for $u \in L^2(\gamma)$. A natural way to proceed if we wish to understand this operator is to cover $\mathbf{R}^d$ with a disjoint family of admissible cubes Q and

[2] This is done for $d = 1$ in this reference, but the proof – using the Mehler kernel– easily extends to general d. Of course much more is true– e^{tL} is contractive for such t and p - but this is not important to us here.

write

$$\pi u = \sum_Q \pi(\mathbf{1}_Q u).$$

Now, using integration by parts, we have formally that

$$\pi u = \int_{m(\cdot)}^{\infty} (t^2 L)^{N+1} e^{t^2 L} u \frac{dt}{t} \sim \sum_{k=0}^{N} (m(\cdot)^2 L)^k e^{2m(\cdot)^2 L} (\mathbf{1}_Q u).$$

To prove boundedness one would now need off-diagonal estimates of the form

$$\left(\int_{C_k(B)} |(m(x)^2 L)^N e^{2m(x)^2 L} (\mathbf{1}_B u(x))|^2 \, d\gamma(x) \right)^{1/2} \lesssim e^{-c4^k} \int_B |u| \, d\gamma. \quad (4.2)$$

In the next section we will show this is not even possible for $k = 0$ and $N = 0$.

4.3. Failure of the full L^1–L^p off-diagonal estimates for all $p > 1$

In applications one is often interested in the case where F are the annuli $C_j(B) = 2^{j+1}B \setminus 2^j B$ for $j \geqslant 1$ and $C_0(B) = 2B$ and where $B = B(c_B, r_B)$ is a ball.

In this section we will provide a counterexample to Definition 4.1 where $T_t = e^{tL}$ is the semigroup associated to the Ornstein-Uhlenbeck operator L. Furthermore, we let $\mu = \gamma$ be the Gaussian measure (1.2).

Our counterexample will be for $F = C_1(B)$ where $E = B(c_B, r_B)$ is a maximal admissible ball such that $|c_B| r_B = 1$ for $|c_B| > 1$. We are only interested in small times $t \in (0, 1)$ as is common in for instance the Hardy space theory in [3]

Under these conditions (4.1) becomes

$$\Big(\int_{C_1(B)} |e^{tL}\mathbf{1}_B|^p \,\mathrm{d}\gamma\Big)^{1/p} \lesssim t^{-\theta} \exp\Big(-c\frac{d^2(B,C_1(B))}{t}\Big)\gamma(B), \tag{4.3}$$

where the implicit constant does not depend on t, $C_1(B)$ and B. We will assume that (4.3) holds and derive a contradiction.

As a first step we find a lower bound for $\mathrm{e}^{tL}\mathbf{1}_B$. Recall that

$$\mathrm{e}^{tL}u(x) = \int_{\mathbf{R}^d} M_t(x,y)u(y)\,\mathrm{d}\gamma(y),$$

where M_t is the *Mehler kernel* defined in (1.33).

As we wish to find a lower bound for $\mathrm{e}^{tL}\mathbf{1}_B$ we first proceed with a lower bound for the first exponential on the right-hand side. For $j \geqslant 1$ we have when $y \in C_j(B)$ that

$$2^j r_B < |y - c_B| \leqslant 2^{j+1} r_B.$$

Using the triangle inequality we obtain for $x \in B$:

$$(2^j - 1)r_B < |y - c_B| - |x - c_B| \leqslant |x - y| \leqslant |y - c_B| + |x - c_B| \leqslant (2^{j+1} + 1)r_B.$$

Hence, in the case $j = 1$ we have that $|x - y| \leqslant 5r_B$. Additionally, as $t \in (0,1)$, we see that

$$\frac{1}{t} \leqslant \frac{1}{1-\mathrm{e}^{-t}} \leqslant \frac{2}{t}.$$

Which follows from

$$\mathrm{e}^{-t} = 1 - t + \frac{t^2}{2!} + O(t^3).$$

Or that,

$$\frac{1}{t} \leqslant \frac{1}{1-\mathrm{e}^{-t}} \leqslant \frac{1}{t}(1 - t/2)^{-1} \leqslant \frac{2}{t},$$

So that

$$e^{tL}\mathbf{1}_B(x) \geqslant t^{-d/2}\exp\Big(-\frac{5^2 r_B^2}{t}\Big)\int_B \exp\Big(2e^{-t}\frac{\langle x,y\rangle}{1+e^{-t}}\Big)\,d\gamma(y). \qquad (4.4)$$

In the next step we will find a lower bound on $\langle x,y\rangle = |x||y|\cos\theta_{x,y}$ where $\theta_{x,y}$ is the angle between the vectors $x \in B$ and $y \in C_1(B)$. We will assume from now on that $|c_B| > 4$. Then $r_B < \frac{1}{4}$ and the angle between x and y is smaller than $\pi/2$. In the end we will derive a contradiction when $|c_B| \to \infty$. So, in the case that $|c_B| > 4$, we can see that $|x| \geqslant |c_B| - r_B$ and $|y| \geqslant |c_B| - 4r_B$. Pick $\varepsilon_{t,p} = \varepsilon > 0$ such that

$$1 - \varepsilon_{t,p} > \frac{e^t + 1}{2p} \geqslant \frac{1}{p}.$$

Note that we can only have $\varepsilon > 0$ if $p > 1$. As the problem is rotationally invariant, we can rotate x, y and c_B such that $c_B = |c_B|e_1$ where e_1 is the first unit vector, then the angle is certainly smaller than the angle between the vector $x_0 := c_B$ and the vector $y_0 := c_B + 4r_B e_i$ where $e_1 \cdot e_i = 0$. This situation is shown in Figure 4.1 Thus, using that $|c_B|r_B = 1$ and $r_B \leqslant \frac{1}{4}$,

$$\sup_{\substack{x\in B\\ y\in C_1(B)}} \cos\theta_{x,y} \geqslant \cos\theta_{x_0,y_0} \geqslant \Big(\frac{|c_B|^2}{|c_B|^2 + 16r_B^2}\Big)^{1/2} = \Big(\frac{1}{1+16r_B^4}\Big)^{1/2}.$$

If we take $|c_B| > 2/(p^2-1)^{1/4}$ then $r_B < \frac{(p^2-1)^{1/4}}{2}$ so that

$$\Big(\frac{1}{1+16r_B^4}\Big)^{1/2} > \Big(\frac{1}{1+(p^2-1)}\Big)^{1/2} \geqslant \frac{1}{p}.$$

Hence, we have that $\cos\theta_{x,y} \geqslant 1-\varepsilon$ for all $x \in B$ and $y \in C_1(B)$. Using

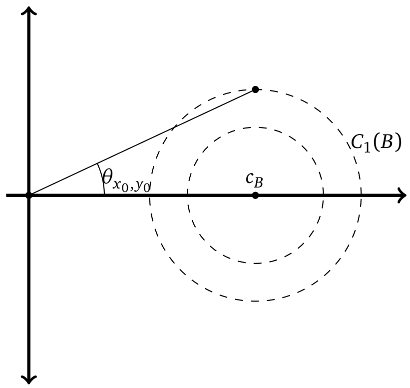


Figure 4.1.: Graphical representation of the angle θ_{x_0,y_0}.

that $\cos\theta_{x,y} \geqslant 1-\varepsilon$, we get that

$$\begin{aligned}\langle x, y\rangle &= |x||y|\cos\theta_{x,y}\\ &\geqslant (|c_B|-r_B)(|c_B|-4r_B)(1-\varepsilon)\\ &\geqslant |c_B|^2(1-\varepsilon)-5(1-\varepsilon).\end{aligned}$$

Therefore, for all $x \in B$ and $y \in C_1(B)$

$$\exp\Big(2\mathrm{e}^{-t}\frac{\langle x, y\rangle}{1+\mathrm{e}^{-t}}\Big) \geqslant_{t,p} \exp\Big(2\frac{|c_B|^2(1-\varepsilon)}{\mathrm{e}^t+1}\Big).$$

From (4.4) we conclude that

$$\mathrm{e}^{tL}\mathbf{1}_B(x) \gtrsim t^{-d/2}\exp\Big(-\frac{5^2 r_B^2}{t}\Big)\exp\Big(2\frac{|c_B|^2(1-\varepsilon)}{\mathrm{e}^t+1}\Big)\gamma(B).$$

As we have assumed (4.3) holds, then

$$\exp\Big(-\frac{5^2 r_B^2}{t}\Big)\exp\Big(2\frac{|c_B|^2(1-\varepsilon)}{\mathrm{e}^t+1}\Big)\gamma(C_1(B))^{1/p} \lesssim_{t,p} \exp\Big(-c\frac{r_B^2}{t}\Big).$$

should hold as well. As a final step we lower bound $\gamma(C_1(B))$

$$\begin{aligned}\gamma(C_1(B)) &\simeq_d \int_{C_1(B)} \mathrm{e}^{-|x|^2}\,dx \\ &\geqslant |C_1(B)|\mathrm{e}^{-(|c_B|+4r_B)^2} \\ &\simeq_d r_B^d|B(0,1)|\mathrm{e}^{-|c_B|^2}\mathrm{e}^{-8|c_B|r_B}\mathrm{e}^{-16r_B^2}.\end{aligned}$$

Using that $|c_B|r_B = 1$ we obtain

$$\gamma(C_1(B))^{1/p} \gtrsim_d |c_B|^{-d/p}\mathrm{e}^{-\frac{1}{p}|c_B|^2}.$$

Combining the above two estimates we get for a $c' \geqslant 0$ that

$$\exp\Big(\Big[2\frac{(1-\varepsilon)}{\mathrm{e}^t+1} - \frac{1}{p}\Big]|c_B|^2\Big) \lesssim_t |c_B|^{d/p}\exp\Big(c'\frac{r_B^2}{t}\Big). \tag{4.5}$$

For fixed t we can bound the term on the right-hand side by $|c_B|^{d/p}$. Due to the choice of ε, the coefficient of $|c_B|^2$ in the exponential is positive, hence we have a $c'' > 0$ such that

$$\mathrm{e}^{c''|c_B|^2} \lesssim_t |c_B|^{d/p}.$$

Which is certainly false for $|c_B| \to \infty$. In conclusion, whenever $F = C_j(B)$ and $E = B$ where B is maximally admissible, the off-diagonal estimates (4.3) can never hold for the Ornstein-Uhlenbeck operator in the local range $t \in (0,1)$.

However, in the motivation to this chapter we wish to have off-diagonal estimates of the form (4.2) which are slightly weaker than the ones we have just disproven. In the motivation we have $t = m(x)^2$, but Lemma 2.1 combined with $|x - c_B| \leqslant r_B = m(c_B)$ and $|y - c_B| \leqslant 4r_B$ implies that

$$m(x) \sim m(y) \sim m(c_B).$$

From this we can conclude that $r_B^2 \sim t$, and by virtue of (4.5) this implies that (4.2) also does not hold in this case.

4.4. Acknowledgments

The author would like to thank Mikko Kemppainen for suggesting this problem.

References

[1] Pascal Auscher and José Maria Martell. "Weighted norm inequalities, off-diagonal estimates and elliptic operators. Part I: General operator theory and weights". In: (2006). eprint: `arXiv:math/0603640` (see p. 70).

[2] Alexander Grigor'yan. *Heat kernel and analysis on manifolds.* English. Providence, RI: American Mathematical Society (AMS); Somerville, MA: International Press, 2009, xvii + 482 (see p. 70).

[3] Giancarlo Mauceri and Stefano Meda. "BMO and H^1 for the Ornstein–Uhlenbeck operator". In: *Journal of Functional Analysis* 252.1 (Nov. 2007), 278–313. DOI: `10.1016/j.jfa.2007.06.017` (see pp. 71, 73).

[4] Edward Nelson. "A quartic interaction in two dimensions". In: *Mathematical Theory of Elementary Particles (Proc. Conf., Dedham, Mass., 1965)*. M.I.T. Press, Cambridge, Mass., 1966, 69–73 (see p. 71).

[5] Pierre Portal and Jan van Neerven. "Finite speed of propagation and off-diagonal bounds for Ornstein-Uhlenbeck operators in infinite dimensions". In: (2015). eprint: `arXiv:1507.02082` (see p. 71).

[6] Peter Sjögren. “Operators associated with the Hermite semigroup—a survey”. In: *Proceedings of the conference dedicated to Professor Miguel de Guzmán (El Escorial, 1996)*. Vol. 3. Special Issue. 1997, 813–823. DOI: 10.1007/BF02656487 (see p. 70).

[7] Jonas Teuwen. “A note on Gaussian maximal functions”. In: *Indagationes Mathematicae* 26.1 (2015), 106–112. DOI: 10.1016/j.indag.2014.07.017 (see p. 70).

II.

Physics

5. Optimizing the electric energy density in a disc

In this chapter we study the electric field which optimizes the energy density in a given disc. Using the Lagrange multiplier rule for infinite-dimensional spaces we derive an integral equation for the optimum amplitudes of the field. Using these, we look at the fields in the entrance pupil and in the focal point where the disc radiuses are in the order of magnitude of the wave length of the incident light.

5.1. Introduction

In this chapter we consider a disk centered at the origin with radius R where we compute the electric field which has maximal energy density in this disk under the constraint of fixed numerical aperture.

To do this we set up an expansion of the electric field in term of plane waves. We can apply the Kuhn-Tucker rule for infinite-dimensional problems to this expansion to obtain an integral equation for the amplitudes of these plane waves.

Finally, we compute the fields in the entrance pupil and the focal point.

5.2. The necessary ingredients

5.2.1. The electric and magnetic field in terms of plane wave amplitudes

We start with by introducing the notation. Consider a time-harmonic electromagnetic field in a homogeneous unbounded medium, the refractive index n is real and the electromagnetic field is given by

$$\mathscr{E}(\mathbf{r},t) = \mathrm{Re}[\mathbf{E}(\mathbf{r})\mathrm{e}^{-i\omega t}], \tag{5.1}$$

and

$$\mathscr{H}(\mathbf{r},t) = \mathrm{Re}[\mathbf{H}(\mathbf{r})\mathrm{e}^{-i\omega t}]. \tag{5.2}$$

where the frequency $\omega > 0$. We will assume that with respect to the Cartesian coordinates (x, y, z) with unit vectors $\widehat{\mathbf{x}}, \widehat{\mathbf{y}}$ and $\widehat{\mathbf{z}}$ the electromagnetic field as in (5.1) and (5.2) has numerical aperture $\mathrm{NA} \leqslant n$ and is propagating in the positive z-direction. So, we write the electric field into a plane wave expansion as

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi^2} \iint_{\sqrt{k_x^2+k_y^2} \leqslant k_0 \mathrm{NA}} \mathbf{A}(k_x, k_y) e^{i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{k}_{\|}, \tag{5.3}$$

where $k_0 = \omega\sqrt{\varepsilon_0\mu_0}$ and where we have abbreviated $(k_x, k_y, 0)$ by $\mathbf{k}_{\|}$. Note that there are no the evanescent waves in this expansion. The vector $\mathbf{k}$ is defined as

$$\mathbf{k} := \mathbf{k}_{\|} + k_z\widehat{\mathbf{z}}, \text{ with } k_z := \sqrt{k^2 - (k_x^2 + k_y^2)},$$

where $k = k_0 n = \omega\sqrt{\varepsilon_0\mu_0}n$. Faraday's law $\nabla \times \mathbf{E} = -\partial_t \mathbf{B}$ implies that the magnetic field $\mathbf{H}$ can be written as

$$\mathbf{H}(\mathbf{r}) = \frac{1}{\omega\mu_0} \frac{1}{4\pi^2} \iint_{\sqrt{k_x^2+k_y^2} \leqslant k_0 \mathrm{NA}} \mathbf{k} \times \mathbf{A}(k_x, k_y) e^{i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{k}_{\|}. \tag{5.4}$$

For convenience we will define Ω as

$$\Omega := \left\{(k_x, k_y) : \sqrt{k_x^2 + k_y^2} \leqslant k_0 \mathrm{NA}\right\}. \tag{5.5}$$

The numerical aperture is given by $\mathrm{NA} = n \sin \alpha_{\max}$ where $\alpha_{\max}$ is the maximum angle that the wave vectors make with the positive z-axis.

Because the electric field is divergence free, we have

$$\nabla \cdot \mathbf{E}(\mathbf{r}) = \frac{1}{4\pi^2} \iint_{\Omega} \mathbf{A}(\mathbf{k}_{\|}) \cdot \nabla e^{i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{k}_{\|} = \frac{1}{4\pi^2} \iint_{\Omega} \mathbf{A}(\mathbf{k}_{\|}) \cdot \mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} \, d\mathbf{k}_{\|} = 0.$$

As this holds for all electric fields, we can conclude

$$\mathbf{A} \cdot \mathbf{k} = 0.$$

To reduce the number of degrees of freedom for $\mathbf{A}$ we will use spherical coordinates in reciprocal $\mathbf{k}$-space, more precisely we use the basis

$$\widehat{\mathbf{s}}(\mathbf{k}) = \frac{1}{|\mathbf{k}_{||}|}\begin{pmatrix} k_y \\ -k_x \\ 0 \end{pmatrix}, \text{ and, } \widehat{\mathbf{p}}(\mathbf{k}) = \frac{1}{k}\frac{1}{|\mathbf{k}_{||}|}\begin{pmatrix} -k_x k_z \\ -k_y k_z \\ k_x^2 + k_y^2 \end{pmatrix}.$$

Note that $(\widehat{\mathbf{k}}, \widehat{\mathbf{p}}, \widehat{\mathbf{s}})$ is a *positively oriented orthonormal basis* in the sense that $\widehat{\mathbf{k}} \times \widehat{\mathbf{p}} = \widehat{\mathbf{s}}$. Because $\mathbf{A} \cdot \mathbf{k} = 0$ we can write

$$\mathbf{A}(k_x, k_y) = A_P(k_x, k_y)\widehat{\mathbf{p}}(k_x, k_y) + A_S(k_x, k_y)\widehat{\mathbf{s}}(k_x, k_y),$$

where A_P is the component parallel to the plane through the wave vector and the z-axis and A_S is perpendicular *("senkrecht")* to this plane.

The time-average power flow is given by the integral over a plane plane $z =$ constant of the time-average of the complex Poynting vector $\mathbf{S} = \mathbf{E} \times \mathbf{H}^*$ and is given by [11, Equation 24]:

$$P(\mathbf{E}, \mathbf{H}) = \iint_{\mathbf{R}^2} \frac{1}{2} \operatorname{Re}\{\mathbf{S}(\mathbf{r})\} \cdot \widehat{\mathbf{z}} \, \mathrm{d}x \, \mathrm{d}y, \tag{5.6}$$

Note that, since there is no absorption, the integral (5.6) is independent on the precise choice of the plane $z =$ constant. Using Plancherel's theorem together with $\mathbf{A} \cdot \mathbf{k} = 0$, we get as in [11, Equation 25] that the power flow (5.6) can be expressed in the amplitudes of the plane waves by:

$$\begin{aligned} P(\mathbf{A}) &= \frac{1}{\omega\mu_0}\frac{1}{8\pi^2}\iint_{\Omega} |\mathbf{A}(k_x, k_y)|^2 k_z \, \mathrm{d}\mathbf{k}_{||} \\ &= \frac{1}{\omega\mu_0}\frac{1}{8\pi^2}\langle k_z, |\mathbf{A}|^2\rangle_{L^2(\Omega)}. \end{aligned} \tag{5.7}$$

5.2.2. The optimization functional

We want to maximize the electric energy density in a disk centered in the plane $z = 0$ for time-harmonic electromagnetic fields that propagate in the positive z-direction and have given total power flow in the positive z-direction and of which the wave vectors in the plane wave expansion are constraint by the specified numerical aperture. Later, in Section 5.5 we will consider how such an field can be realized by focusing an appropriate pupil field using a lens with the mentioned numerical aperture.

The time-averaged electric energy in the disc D in the plane $z = 0$, with the centre the origin and radius R is given by

$$F(\mathbf{E},R) := F(R) := \frac{1}{|D|}\iint_D |\mathbf{E}|^2 \,\mathrm{d}x\mathrm{d}y = \frac{1}{|D|}\langle \mathbf{E}1_D, \mathbf{E}\rangle_{L^2(\mathbf{R}^2)}. \tag{5.8}$$

Here 1_D is the indicator of D, that is $1_D(\mathbf{r}) = 1$ if $\mathbf{r}$ is in D and else 0.

Because it turns out to be convenient to formulate the optimization problem in terms of the plane wave amplitudes A_P and A_S we use the Fourier transform and Parseval's formula. We will use the Fourier normalization (5.46) with inverse (5.47). Proceeding, we use the convolution identity (5.48) to rewrite (5.8)

$$F(\mathbf{E},R) = \frac{1}{|D|}\langle \mathbf{E}1_D, \mathbf{E}\rangle_{L^2(\mathbf{R}^2)} = \frac{1}{|D|}\frac{1}{4\pi^2}\langle \mathscr{F}(\mathbf{E}) * \mathscr{F}(1_D), \mathscr{F}(\mathbf{E})\rangle_{L^2(\mathbf{R}^2)}. \tag{5.9}$$

We introduce the notation

$$C_R(k_x,k_y) := \frac{1}{4\pi^2}\frac{1}{|D|}\mathscr{F}(1_D)(k_x,k_y) = \frac{1}{2\pi^2}\frac{J_1\left(R\sqrt{k_x^2+k_y^2}\right)}{R\sqrt{k_x^2+k_y^2}}. \tag{5.10}$$

So, we can write (5.9) as

$$F(\mathbf{E},R) = \langle \mathscr{F}(\mathbf{E}) * C_R, \mathscr{F}(\mathbf{E})\rangle_{L^2(\mathbf{R}^2)}. \tag{5.11}$$

This leads us with a slight abuse of notation that (5.11) is equal to

$$F(\mathbf{A},R) := \langle \mathbf{A} * C_R, \mathbf{A} \rangle_{L^2(\Omega)} = \iint_\Omega (\mathbf{A} * C_R)(\mathbf{k}_{\|})\mathbf{A}(\mathbf{k}_{\|})^* \, \mathrm{d}\mathbf{k}_{\|}. \quad (5.12)$$

Note that the present method generalizes to more general geometries different from the disk as the only place where the disk occurs is when we take the Fourier transform of its indicator to obtain the function C_R.

5.3. The optimum plane wave amplitudes

5.3.1. The abstract optimization problem

We consider the L^2-space $\mathscr{H}$ as the Hilbert space with norm $\|\cdot\|_{\mathscr{H}} := \sqrt{\langle\cdot,\cdot\rangle_{\mathscr{H}}}$. This space $\mathscr{H}$ is defined as

$$\mathscr{H} := \{\mathbf{A} = (A_P, A_S) : \Omega \to \mathbb{C}^2 : \|\mathbf{A}\|_{\mathscr{H}} < \infty\}.$$

This is a Hilbert space as it is a closed subspace of $L^2(\mathbf{R}^2)$. The norm is induced by the inner product by $\|\cdot\| := \sqrt{\langle\cdot,\cdot\rangle}$ where the inner product is the usual $L^2(\mathbf{R}^d)$ inner product. On any basis this inner product can be written as

$$\langle \mathbf{A}, \mathbf{B} \rangle = \iint_\Omega \mathbf{A} \cdot \mathbf{B}^* \, \mathrm{d}\mathbf{k}_{\|}.$$

We are now in the position to define the set $\mathscr{B}$ in which the solutions is sought. This is a closed subset of $\mathscr{H}$ which is given a maximal power flow P_0 given by

$$\mathscr{B} := \{\mathbf{A} \in \mathscr{H} : P(\mathbf{A}) \leqslant P_0\}.$$

The optimization problem is now given a power $P_0 \geqslant 0$ to find a (not necessarily unique) $\mathbf{A} \in \mathscr{B}$ such that $F(\mathbf{A}, R)$ is *maximal*. Note that for any such solution $\mathbf{A}$ we would actually have $P(\mathbf{A}) = P_0$, because otherwise $\mathbf{A}$ could be multiplied by $(P_0/P(\mathbf{A}))^{\frac{1}{2}} > 1$ and we would obtain a better $\mathbf{A}$. The equality constraint $P(\mathbf{A}) = P_0$ would thus define an equivalent problem, but this contraint does define a convex set which would be less convenient from a mathematical point of view.

In what follows, we will solve this optimization problem using the Lagrange multiplier rule for inequality constraints, the so-called Kuhn-Tucker theorem. For our problem the Kuhn-Tucker theorem [7, Theorem p.249] states that:

> There exists a Lagrange multiplier $\Lambda' \geqslant 0$ such that if $\mathbf{A}$ is the optimum field we have that
>
> $$\delta F(\mathbf{A})(\mathbf{B}) - \Lambda' \delta P(\mathbf{A})(\mathbf{B}) = 0 \text{ for all } \mathbf{B} \text{ in } \mathscr{H}. \tag{5.13}$$

Here $\delta F(\mathbf{A})(\mathbf{B})$ is the *Gateaux derivative* of F at $\mathbf{A}$ in the direction of $\mathbf{B}$, which is given by

$$\delta F(\mathbf{A})(\mathbf{B}) := \lim_{t \to 0} \frac{1}{t} [F(\mathbf{A} + t\mathbf{B}) - F(\mathbf{A})]. \tag{5.14}$$

and similarly for $\delta P(\mathbf{A})(\mathbf{B})$. The derivatives δF and δP can be compute directly from the definition (5.14). For F, given in (5.8) we find:

$$\begin{aligned}\delta F(\mathbf{A})(\mathbf{B}) &= \lim_{t\to 0}\frac{1}{t}[F(\mathbf{A}+t\mathbf{B})-F(\mathbf{A})]\\ &= \lim_{t\to 0}\frac{1}{t}[t\langle C_R*\mathbf{A},\mathbf{B}\rangle + t\langle C_R*\mathbf{B},\mathbf{A}\rangle + t^2\langle C_R*\mathbf{B},\mathbf{B}\rangle]\\ &= 2\,\mathrm{Re}\{\langle C_R*\mathbf{A},\mathbf{B}\rangle\}.\end{aligned}$$

Similarly we can compute the Gateaux derivative for P as given in (5.7). For this we use the expansion

$$|\mathbf{A}+t\mathbf{B}|^2 = |\mathbf{A}|^2 + 2t\,\mathrm{Re}\{\mathbf{A}\cdot\mathbf{B}\} + t^2|\mathbf{B}|^2,$$

where $\mathbf{A}\cdot\mathbf{B}$ is the Euclidean inner product between $\mathbf{A}$ and $\mathbf{B}$. Concluding we see that the Gateaux derivatives of F and P in $\mathbf{A}$ in the direction of $\mathbf{B}$ are given by,

$$\delta F(\mathbf{A})(\mathbf{B}) = 2\,\mathrm{Re}\langle (C_R*\mathbf{A}),\mathbf{B}\rangle_{L^2(\Omega)}, \tag{5.15}$$

$$\delta P(\mathbf{A})(\mathbf{B}) = 2\frac{1}{\omega\mu_0}\frac{1}{8\pi^2}\,\mathrm{Re}\langle \mathbf{A}k_z,\mathbf{B}\rangle_{L^2(\Omega)}. \tag{5.16}$$

So, (5.13) together with (5.15) and (5.16) gives

$$\mathrm{Re}\langle C_R*\mathbf{A},\mathbf{B}\rangle_{L^2(\Omega)} - \Lambda\,\mathrm{Re}\langle \mathbf{A}k_z,\mathbf{B}\rangle_{L^2(\Omega)} = 0$$

for all $\mathbf{B}$ in $\mathscr{H}$. Where

$$\Lambda = \frac{1}{\omega\mu_0}\frac{1}{8\pi^2}\Lambda'.$$

Equation 5.3.1 implies

$$\mathrm{Re}\langle C_R*\mathbf{A}-\Lambda\mathbf{A}k_z,\mathbf{B}\rangle_{L^2(\Omega)} = 0, \tag{5.17}$$

Define

$$T\mathbf{A} := \frac{C_R*\mathbf{A}}{k_z}. \tag{5.18}$$

Then, for the optimal $\mathbf{A}$, there would hold that:

$$\Lambda \mathbf{A} = T\mathbf{A}, \tag{5.19}$$

in Ω. Hence $\mathbf{A}$ is an eigenfield of the operator T and Λ is its corresponding eigenvalue.

Note that when $\mathbf{A}_{\text{opt}}$ is the optimum field then

$$F(\mathbf{A}_{\text{opt}}) = \frac{1}{2}\delta F(\mathbf{A}_{\text{opt}})(\mathbf{A}_{\text{opt}}),$$
$$P(\mathbf{A}_{\text{opt}}) = \frac{1}{2}\delta P(\mathbf{A}_{\text{opt}})(\mathbf{A}_{\text{opt}}).$$

Substituting into (5.13), we can see that the maximal eigenvalue Λ'_{max} and the maximal power density are related by

$$F_{\text{opt}} = \Lambda'_{\text{max}} P_0. \tag{5.20}$$

In the next section we derive several mathematical properties of the mathematical problem which will provide us of information without computing the solution.

5.4. Mathematical properties of the operator T

In this section we derive some properties of the model without explicitly computing the solution, as this will be done numerically in the next section. We will show that the eigenvalues are all real and positive, which is consistent with the fact that according to (5.20) these eigenvalues are the ratio of two positive quantities, namely the total electric energy in the disc and the power flow of P_0. We will also introduce a spherical coordinate system to be able to reduce the number of variables in direct computations.

5.4.1. The operator T is Hilbert-Schmidt

In this section we will show that the operator T as defined in (5.18) is *Hilbert-Schmidt*. This class of operators plays an important role in many problems of mathematical physics. For the problem at hand the most important properties of a Hilbert-Schmidt operator are the fact that the eigenfields and eigenvalues form a *discrete set* and that there is a largest eigenvalue which can be estimated from above using the the kernel of the operator.

Considering this operator T:

$$T(\mathbf{A}) := \iint_{\mathbf{R}^2} K(\mathbf{k}'_{\|}, \mathbf{k}_{\|}) \, \mathrm{d}\mathbf{k}'_{\|}, \tag{5.21}$$

for $\mathbf{A}$ in $L^2(\Omega)$, where the integral kernel K has support in $\Omega \times \Omega$ and is given by

$$K(\mathbf{k}'_{\|}, \mathbf{k}_{\|}) := C_R(\mathbf{k}'_{\|} - \mathbf{k}_{\|}) \frac{1_{\Omega\times\Omega}(\mathbf{k}'_{\|}, \mathbf{k}_{\|})}{\sqrt{k^2 - |\mathbf{k}_{\|}|^2}}. \tag{5.22}$$

By [8, Theorem VI.22] the operator T is Hilbert-Schmidt if and only if the kernel is square integrable. This means that we need to verify that

$$\|K\|^2_{L^2(\mathbf{R}^2\times\mathbf{R}^2)} = \int_\Omega \int_\Omega \frac{C_R(\mathbf{k}'_{\|} - \mathbf{k}_{\|})^2}{k^2 - |\mathbf{k}_{\|}|^2} \, \mathrm{d}\mathbf{k}'_{\|} \, \mathrm{d}\mathbf{k}_{\|} < \infty.$$

On Ω we can bound this integral above by

$$\frac{1}{k^2 \cos^2 \alpha_{\max}} \int_\Omega \int_\Omega C_R(\mathbf{k}'_{\|} - \mathbf{k}_{\|})^2 \, \mathrm{d}\mathbf{k}'_{\|} \, \mathrm{d}\mathbf{k}_{\|} = \frac{|\Omega| \|C_R\|^2_{L^2(\mathbf{R}^2)}}{k^2 \cos^2 \alpha_{\max}}.$$

As $|\Omega| = \pi k^2 \sin^2 \alpha_{\text{max}}$, we only need an upper bound for $\|C_R\|_{L^2(\mathbf{R}^2)}$. By Parseval's formula (5.49) we know that

$$\|C_R\|^2_{L^2(\mathbf{R}^2)} = \frac{1}{(4\pi^2)^2} \frac{1}{|D|^2} \|\widehat{1_D}\|^2_{L^2(\mathbf{R}^2)} = \frac{1}{4\pi^2} \frac{1}{|D|^2} \|1_D\|^2_{L^2(\mathbf{R}^2)} = \frac{1}{4\pi^2} \frac{1}{|D|}.$$

Hence, for $\alpha_{\text{max}} < \frac{\pi}{2}$ the operator T is Hilbert-Schmidt. The case $\alpha_{\text{max}} = \frac{\pi}{2}$ requires a different argument. It implies that $\text{NA}/n = 1$ which is a case which we will not use. For the L^2-norm we have

$$\|K\|^2_{L^2(\mathbf{R}^2 \times \mathbf{R}^2)} \leqslant \frac{\pi k^2 \sin^2 \alpha_{\text{max}}}{k^2 \cos^2 \alpha_{\text{max}}} \frac{1}{4\pi^2} \frac{1}{|D|} = \frac{\tan^2 \alpha_{\text{max}}}{4\pi^2 R^2}.$$

As the operator is Hilbert-Schmidt, it is compact hence has a discrete spectrum [8, Theorem VI.17]. The modulus of the largest eigenvalue of a Hilbert-Schmidt operator is equal to the operator norm. Since Λ_{max} is positive, we can deduce that

$$0 \leqslant \Lambda_{\text{max}} \leqslant \frac{\tan \alpha_{\text{max}}}{2\pi R}.$$

We remark that if the electromagnetic field is realized by focusing with a lens with numerical aperture NA and a focal lens f, then the radius of the aperture of the lens is $R_{\text{lens}} = f \sin \alpha_{\text{max}}$ and hence

$$\Lambda_{\text{max}} \leqslant \frac{R_{\text{lens}}}{2Rf\,\pi \cos \alpha_{\text{max}}} = \frac{R_{\text{lens}}}{2\pi Rf} \frac{1}{\sqrt{1 - \frac{\text{NA}^2}{n^2}}}.$$

It follows from the Kuhn-Tucker condition (5.13) that the maximal eigenvalue is positive and real. For our operator T this a is a more general fact about *all* eigenvalues. To see this we test T in (5.21) against a function $\mathbf{B}$. As a first step, we rewrite (5.17) as

$$\Lambda \langle k_z \mathbf{A}, \mathbf{B} \rangle = \langle C_R * \mathbf{A}, \mathbf{B} \rangle. \tag{5.23}$$

Taking complex conjugates in this expression we obtain that

$$\Lambda^* \langle \mathbf{A}, k_z \mathbf{B} \rangle = \langle \mathbf{A}, C_R * \mathbf{B} \rangle, \tag{5.24}$$

where we have used that $\langle \mathbf{A}, \mathbf{B} \rangle^* = \langle \mathbf{B}, \mathbf{A} \rangle$. The functions k_z and C_R are real, hence the operators $\mathbf{A} \mapsto k_z \mathbf{A}$ and $\mathbf{A} \mapsto C_R * \mathbf{A}$ are self-adjoint. This means that

$$\langle \mathbf{A}, k_z \mathbf{B} \rangle = \langle k_z \mathbf{A}, \mathbf{B} \rangle \text{ and, } \langle \mathbf{A}, C_R * \mathbf{B} \rangle = \langle C_R * \mathbf{A}, \mathbf{B} \rangle$$

for all **A** and **B**. Hence, (5.24) reduces to

$$\Lambda^* \langle k_z \mathbf{A}, \mathbf{B} \rangle = \langle C_R * \mathbf{A}, \mathbf{B} \rangle, \tag{5.25}$$

Comparing (5.23) with (5.25), we can conclude that $\Lambda = \Lambda^*$ or that all eigenvalues Λ of T are real. For the positivity, we can note that T is a positive operator as C_R and k_z are positive functions.

5.4.2. Decoupling the angular term

To make use of the rotational symmetry in the lens we introduce a spherical coordinate system.

Spherical coordinates

We will solve the optimization problem (5.19) by writing the integral equation in spherical coordinates in image space. The orthonormal $(\widehat{\mathbf{k}}, \widehat{\mathbf{p}}, \widehat{\mathbf{s}})$-basis from above can be written as

$$\widehat{\mathbf{k}}(\alpha,\beta) = \begin{pmatrix} \sin\alpha\cos\beta \\ \sin\alpha\sin\beta \\ \cos\alpha \end{pmatrix},$$

$$\widehat{\mathbf{p}}(\alpha,\beta) = \begin{pmatrix} -\cos\alpha\cos\beta \\ -\cos\alpha\sin\beta \\ \sin\alpha \end{pmatrix}, \tag{5.26}$$

$$\widehat{\mathbf{s}}(\beta) = \begin{pmatrix} \sin\beta \\ -\cos\beta \\ 0 \end{pmatrix},$$

with $\mathbf{k} = k\widehat{\mathbf{k}}$, and where α is the polar angle with $0 \leqslant \alpha \leqslant \alpha_{\max}$ and β the azimuthal angle with $0 \leqslant \beta \leqslant 2\pi$.

We will write all integrals over $\mathbf{k}_{||}$ in terms of integrals over α and β. To do this, we need the Jacobian J of the transformation $(\alpha,\beta) \mapsto (k_x,k_y)$, which is given by

$$\mathrm{d}k_x\,\mathrm{d}k_y = k_0^2 n^2 \cos\alpha\sin\alpha\,\mathrm{d}\alpha\,\mathrm{d}\beta = k^2\cos\alpha\sin\alpha\,\mathrm{d}\alpha\,\mathrm{d}\beta.$$

We will also write this as

$$\mathrm{d}k_x\,\mathrm{d}k_y = \mathrm{d}\,\nu(\alpha)\,\mathrm{d}\beta,$$

when simplicity dictates. Due to rotational symmetry we can write the integration domain Ω from (5.5) in terms of α and β as

$$\Omega = \{(\alpha,\beta) : 0 \leqslant \alpha \leqslant \alpha_{\max},\ 0 \leqslant \beta \leqslant 2\pi\}.$$

For instance, in the $(\widehat{\mathbf{k}}, \widehat{\mathbf{p}}, \widehat{\mathbf{s}})$-basis, we can write the expansion of the electric field $\mathbf{E}$ as given by (5.3) as

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{\alpha_{\max}} (A_P \widehat{\mathbf{p}} + A_S \widehat{\mathbf{s}}) e^{i\mathbf{k}\cdot\mathbf{r}} k^2 \cos\alpha \sin\alpha \, \mathrm{d}\alpha \, \mathrm{d}\beta .$$

With a slight abuse of notation we will write $A_S(\alpha, \beta)$ and $A_P(\alpha, \beta)$ when we mean $A_S(k_x, k_y)$ and $A_P(k_x, k_y)$ respectively.

The operator kernel (5.22) needs to be transformed into (α, β) coordinates as well. Looking closely at the expression we note that the function C_R in K is given in terms of $|\mathbf{k}_{||} - \mathbf{k}'_{||}|$, which we analyse first.

Using (5.26) we set,

$$k_x = k \sin\alpha \cos\beta, \qquad k_y = k \sin\alpha \sin\beta,$$
$$k'_x = k \sin\alpha' \cos\beta', \qquad k'_y = k \sin\alpha' \sin\beta'.$$

Substituting these into $|\mathbf{k}_{||} - \mathbf{k}'_{||}|^2 = (k_x - k'_x)^2 + (k_y - k'_y)^2$ gives

$$\begin{aligned} |\mathbf{k}_{||} - \mathbf{k}'_{||}|^2 &= k^2[(\sin\alpha\cos\beta - \sin\alpha'\cos\beta')^2 + (\sin\alpha\sin\beta - \sin\alpha'\sin\beta')^2] \\ &= k^2[\sin^2\alpha + \sin^2\alpha' - 2\sin\alpha\sin\alpha'\cos(\beta - \beta')]. \end{aligned} \tag{5.27}$$

From this we can infer that the dependence of $|\mathbf{k}_{||} - \mathbf{k}'_{||}|$ on β and β' is in terms of $\beta - \beta'$. Then (5.10) implies this holds for C_R too. This will be an important observation when we rewrite the problem later on as a convolution.

The eigenvalue problem (5.19) that we are trying to solve can be written (α, β) using angular coordinates as

$$\Lambda \mathbf{A}(\alpha, \beta) = \int_0^{2\pi} \int_0^{\alpha_{\max}} \frac{C_R(\alpha, \alpha', \beta - \beta')}{k \cos\alpha} \mathbf{A}(\alpha', \beta') \, \mathrm{d}\nu(\alpha') \, \mathrm{d}\beta' \tag{5.28}$$

where $\alpha \mapsto \mathbf{A}(\alpha,\beta)$ is supported in $(0,\alpha_{\max})$.

If we expand $\mathbf{A}$ on the $\widehat{\mathbf{p}}$ and $\widehat{\mathbf{s}}$ basis we could compute the three Euclidean components (A_x, A_y, A_z). Instead of this, we will study the A_S and A_P components of this equation separately. In order to do this, the following quantities will be useful.

$$\begin{aligned}
\widehat{\mathbf{p}}(\alpha,\beta)\cdot\widehat{\mathbf{p}}(\alpha',\beta') &= \cos\alpha\cos\alpha'\cos(\beta-\beta') + \sin\alpha\sin\alpha', \\
\widehat{\mathbf{p}}(\alpha,\beta)\cdot\widehat{\mathbf{s}}(\alpha',\beta') &= \cos\alpha\sin(\beta-\beta'), \\
\widehat{\mathbf{s}}(\alpha,\beta)\cdot\widehat{\mathbf{s}}(\alpha',\beta') &= \cos(\beta-\beta').
\end{aligned}$$

In particular this gives us that

$$\begin{aligned}
\mathbf{A}(\alpha',\beta')\cdot\widehat{\mathbf{p}}(\alpha,\beta) = {} & A_P(\alpha',\beta')[\cos\alpha\cos\alpha'\cos(\beta-\beta') + \sin\alpha\sin\alpha'] \\
& + A_S(\alpha',\beta')\cos\alpha\sin(\beta-\beta'), \\
\mathbf{A}(\alpha',\beta')\cdot\widehat{\mathbf{s}}(\alpha,\beta) = {} & -A_P(\alpha',\beta')\cos\alpha'\sin(\beta-\beta') \\
& + A_S(\alpha',\beta')\cos(\beta-\beta').
\end{aligned}$$

In matrix notation this becomes,

$$\begin{pmatrix} \mathbf{A}(\alpha',\beta')\cdot\widehat{\mathbf{p}}(\alpha,\beta) \\ \mathbf{A}(\alpha',\beta')\cdot\widehat{\mathbf{s}}(\alpha,\beta) \end{pmatrix} = \mathbf{M}(\alpha,\alpha',\beta-\beta') \begin{pmatrix} A_P(\alpha',\beta') \\ A_S(\alpha',\beta') \end{pmatrix}.$$

Where $\mathbf{M}$ is given by

$$\mathbf{M}(\alpha,\alpha',\gamma) = \begin{pmatrix} \cos\alpha\cos\alpha'\cos\gamma + \sin\alpha\sin\alpha' & \cos\alpha\sin\gamma \\ -\cos\alpha'\sin\gamma & \cos\gamma \end{pmatrix} \tag{5.29}$$

Set

$$\mathbf{M}_R(\alpha,\alpha',\gamma) := \frac{k}{\cos\alpha} C_R(\alpha,\alpha',\gamma)\mathbf{M}(\alpha,\alpha',\gamma). \tag{5.30}$$

Then we can write (5.28) componentwise as:

$$\Lambda \begin{pmatrix} A_P(\alpha,\beta) \\ A_S(\alpha,\beta) \end{pmatrix} = \int_0^{2\pi} \int_0^{\alpha_{\max}} \mathbf{M}_R(\alpha,\alpha',\beta-\beta') \begin{pmatrix} A_P(\alpha',\beta') \\ A_S(\alpha',\beta') \end{pmatrix} \times k^2 \sin\alpha' \cos\alpha' \,\mathrm{d}\alpha' \,\mathrm{d}\beta'. \tag{5.31}$$

The integral over β' is a convolution and recalling that $\mathbf{A}$ is supported on the set $(0,\alpha_{\max}) \times (0,2\pi)$ we can rewrite (5.31) as

$$\Lambda \begin{pmatrix} A_P(\alpha,\beta) \\ A_S(\alpha,\beta) \end{pmatrix} = \int_0^{\alpha_{\max}} \left[\mathbf{M}_R(\alpha,\alpha',\cdot) * \begin{pmatrix} A_P(\alpha',\cdot) \\ A_S(\alpha',\cdot) \end{pmatrix} \right](\beta) \,\mathrm{d}\nu(\alpha'). \tag{5.32}$$

Where $*$ is the convolution with respect to β. The fact that (5.32) is written in terms of a convolution over a variable β running from 0 to 2π suggest to expand the functions $\beta \mapsto A_P(\alpha,\beta)$ and $\beta \mapsto A_S(\alpha,\beta)$ for fixed α in terms of a Fourier series.

Letting $\widehat{\mathbf{M}}_R$ be the element-wise Fourier series in β of the matrix $\mathbf{M}_R$, we can compute the Fourier coefficients of $\mathbf{M}_R(\alpha,\alpha',\cdot) * \mathbf{A}(\alpha',\cdot)$ in β by using the convolution theorem in β[1]. This gives us:

$$\left[\mathbf{M}_R(\alpha,\alpha',\cdot) * \begin{pmatrix} A_P(\alpha',\cdot) \\ A_S(\alpha',\cdot) \end{pmatrix} \right]^{\widehat{}} = \widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) \begin{pmatrix} \widehat{A}_P(\alpha',\ell) \\ \widehat{A}_S(\alpha',\ell) \end{pmatrix}.$$

Substituting into (5.32) we get

$$\begin{aligned} &\Lambda \sum_{\ell=-\infty}^{\infty} \begin{pmatrix} \widehat{A}_P(\alpha,\ell) \\ \widehat{A}_S(\alpha,\ell) \end{pmatrix} \mathrm{e}^{i\ell\beta} \\ &\quad = \sum_{\ell=-\infty}^{\infty} \int_0^{\alpha_{\max}} \widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) \begin{pmatrix} \widehat{A}_P(\alpha',\ell) \\ \widehat{A}_S(\alpha',\ell) \end{pmatrix} \mathrm{e}^{i\ell\beta} \,\mathrm{d}\nu(\alpha'). \end{aligned} \tag{5.33}$$

[1] Note that this still holds for matrix-valued functions.

Equating coefficients in (5.33) we get

$$\Lambda \begin{pmatrix} \widehat{A}_P(\alpha,\ell) \\ \widehat{A}_S(\alpha,\ell) \end{pmatrix} = \int_0^{\alpha_{\max}} \widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) \begin{pmatrix} \widehat{A}_P(\alpha',\ell) \\ \widehat{A}_S(\alpha',\ell) \end{pmatrix} \mathrm{d}\nu(\alpha') \tag{5.34}$$

for all ℓ. Letting $\beta \to \beta - \psi$ shows us that the solution will certainly not be unique, but that a rotation over any angle will give us a solution as well. Note that we can assume the solution $(A_P, A_S)^{\mathrm{T}}$ to be real. To see this, we take complex conjugates in (5.28),

$$\Lambda \begin{pmatrix} A_P(\alpha,\beta) \\ A_S(\alpha,\beta) \end{pmatrix}^* = \int_0^{2\pi} \int_0^{\alpha_{\max}} \frac{C_R(\alpha,\alpha',\beta-\beta')}{k\cos\alpha} \begin{pmatrix} A_P(\alpha',\beta') \\ A_S(\alpha',\beta') \end{pmatrix}^* \mathrm{d}\nu(\alpha')\,\mathrm{d}\beta',$$

and note that $\mathbf{A}^*$ is a solution whenever $\mathbf{A} = (A_P, A_S)^{\mathrm{T}}$ is. Thus, so is $\frac{1}{2}(\mathbf{A} + \mathbf{A}^*) = \operatorname{Re}\mathbf{A}$. Remark that when we decompose in the Fourier basis, we should take the real part of $\mathbf{A}(\alpha,\ell)\mathrm{e}^{i\ell\beta}$ and not just of the amplitudes $(A_P, A_S)^{\mathrm{T}}$. From now on we will assume without loss of generality that the solution is real.

Next we compute the Fourier coefficients of $\mathbf{M}_R$. By (5.30) and we get by the convolution theorem that

$$\widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) = \frac{1}{k\cos\alpha} \sum_{\ell'=-\infty}^{\infty} \widehat{C}_R(\alpha,\alpha',\ell-\ell')\widehat{\mathbf{M}}(\alpha,\alpha',\ell'). \tag{5.35}$$

To complete this computation we compute $\widehat{\mathbf{M}}$ with the use of the following two Fourier integrals:

$$\begin{aligned} \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{i\ell\beta}\cos\beta\,\mathrm{d}\beta &= \frac{1}{2}\delta_{\ell,\pm1}, \\ \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{i\ell\beta}\sin\beta\,\mathrm{d}\beta &= \pm\frac{i}{2}\delta_{\ell,\pm1}. \end{aligned}$$

Using these, and recalling the definition of **M** in (5.29) we have

$$\widehat{\mathbf{M}}(\alpha', \alpha, \ell) = \delta_{\ell,0}\begin{pmatrix} \sin\alpha\sin\alpha' & 0 \\ 0 & 0 \end{pmatrix} + \frac{\delta_{\ell,\pm 1}}{2}\begin{pmatrix} \cos\alpha\cos\alpha' & \pm i\cos\alpha \\ \mp i\cos\alpha' & 1 \end{pmatrix}.$$

So finally we have for (5.35) that:

$$\widehat{\mathbf{M}}_R(\ell) = \frac{1}{k\cos\alpha}[\widehat{C}_R(\ell+1)\widehat{\mathbf{M}}(-1) + \widehat{C}_R(\ell)\widehat{\mathbf{M}}(0) + \widehat{C}_R(\ell-1)\widehat{\mathbf{M}}(1)].$$

where we have surpressed the argument of α and α' for brevity. As we assumed without loss of generality that $\mathbf{A}(\alpha, \beta)$ is real, there would hold that $\widehat{\mathbf{A}}(\alpha, \ell)^* = \widehat{\mathbf{A}}(\alpha, -\ell)$, hence ℓ and $-\ell$ would give the same optimum field. Because of this we can assume that $\ell \geqslant 0$. The solution requires that we know the Fourier coefficients of C_R, which are computed in Section 5.11.

We are looking for the optimal solution, and we have one for each ℓ. Our optimal solution corresponds to the one with the largest eigenvalue Λ as this corresponds to the maximal objective value as shown in (5.20). To this end we provide a method where we can directly compute the value of the eigenvalue for each ℓ without the need to find the solution. We can then obtain iteratively the largest eigenvalue and either use this to compute the optimal solution or to directly obtain the theoretical maximum. This is the subject of the next section. Do keep in mind that solving the integral equation numerically will immediately give us the maximal eigenvalue as well, this just provides an alternative method.

5.4.3. How to obtain the optimal ℓ?

If we wish to obtain the value of Λ in (5.34) without computing the solution we can use again the theory of the Hilbert-Schmidt operators. First of all, we can write $\widehat{\mathbf{M}}$ as:

$$\widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) = \frac{1}{k\cos\alpha}\left\{\begin{pmatrix}\widehat{C}_R(\alpha,\alpha',\ell)\sin\alpha\sin\alpha' & 0\\ 0 & 0\end{pmatrix}\right.$$
$$\left. + \frac{1}{2}\begin{pmatrix}\widehat{C}_+(\alpha,\alpha',\ell)\cos\alpha\cos\alpha' & -i\widehat{C}_-(\alpha,\alpha',\ell)\cos\alpha\\ i\widehat{C}_-(\alpha,\alpha',\ell)\cos\alpha' & \widehat{C}_+(\alpha,\alpha',\ell)\end{pmatrix}\right\},$$

where $\widehat{C}_+(\ell) := \widehat{C}_R(\ell+1)+\widehat{C}_R(\ell-1)$ and $\widehat{C}_-(\ell) := \widehat{C}_R(\ell+1)-\widehat{C}_R(\ell-1)$. The theory of Hilbert-Schmidt operators [8] tells us that the maximal eigenvalue is given by

$$\Lambda_{\max}(\ell) = \left(\iint \|\widehat{\mathbf{M}}_R(\alpha,\alpha',\ell)\|^2_{\ell^2} k^2 \sin\alpha\cos\alpha k^2 \sin\alpha'\cos\alpha' \,\mathrm{d}\alpha\,\mathrm{d}\alpha'\right)^{\frac{1}{2}}.$$

where the integral is taken over the set $[0,\alpha_{\max}]^2$ and where,

$$\|\widehat{\mathbf{M}}_R(\alpha,\alpha',\ell)\|^2_{\ell^2} = \frac{1}{4k^2\cos^2\alpha}[(\widehat{C}_R(\ell)\sin\alpha\sin\alpha' + \widehat{C}_+(\ell)\cos\alpha\cos\alpha')^2$$
$$-\widehat{C}_-(\ell)^2(\cos^2\alpha+\cos^2\alpha') + \widehat{C}_+(\ell)^2],$$

where we have suppressed the argument of α and α' in $\widehat{C}_R$, $\widehat{C}_-$ and $\widehat{C}_-$ for brevity.

5.4.4. The coefficients $\widehat{C}_R$

Until now, we have taken the Fourier coefficients of C_R for granted. These $\widehat{C}_R$ are computed in Section 5.11 and are given by (5.51) for $\ell \geqslant 0$ as

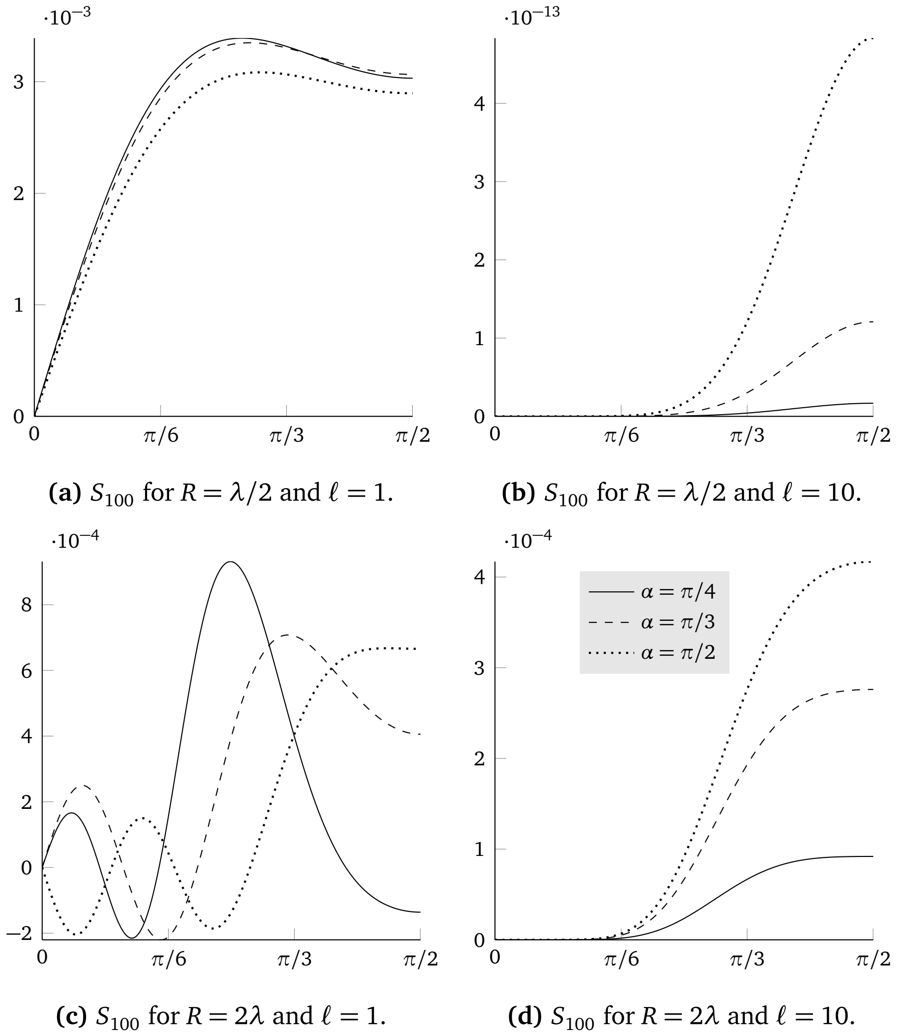
$$\widehat{C}_R(\alpha,\alpha',\ell) := \frac{1}{4\pi^2}\sum_{s=0}^{\infty}\frac{(\sin\alpha\sin\alpha')^{\ell+2s}}{s!(\ell+s)!}\left(\frac{Rk}{\sqrt{2}}\right)^{2\ell+4s} \times \frac{J_{\ell+2s+1}(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})}{(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})^{\ell+2s+1}}.$$

This is a rapidly converging series as can be see in Figure 5.1 for $\ell = 1$. After two terms there is no noticible difference between the series cut off after 100 terms.

5.4.5. Summary of the mathematical properties

For completeness we summarize some of the properties of the solution which we have derived above.

- The eigenvalues Λ are all real and positive.
- The solution $\mathbf{A}$ is not unique, for instance all rotations $\mathbf{A}(\alpha,\beta) \to \mathbf{A}(\alpha,\beta-\psi)$ give feasible solutions.
- There is always a real solution $\mathbf{A}(\alpha,\beta)$.
- In the solution there is only $\ell \geqslant 0$ which matters and the optimum occurs for a single value of ℓ, i.e. the vector $\mathbf{A}(\alpha,\beta)$ depends on β as $e^{\pm i\ell\beta}$.



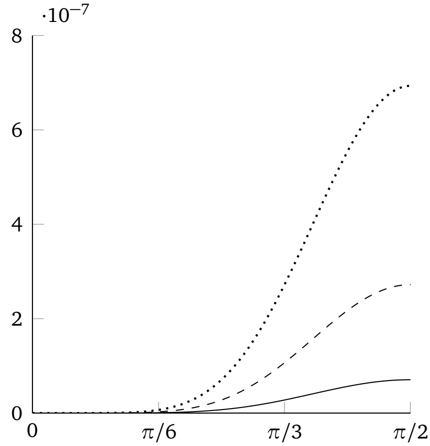
(a) S_{100} for $R = \lambda/2$ and $\ell = 1$.

(b) S_{100} for $R = \lambda/2$ and $\ell = 10$.

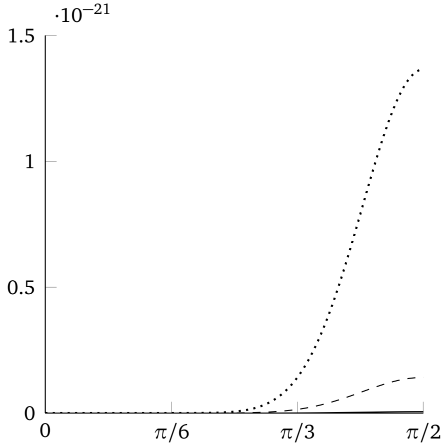
(c) S_{100} for $R = 2\lambda$ and $\ell = 1$.

(d) S_{100} for $R = 2\lambda$ and $\ell = 10$.

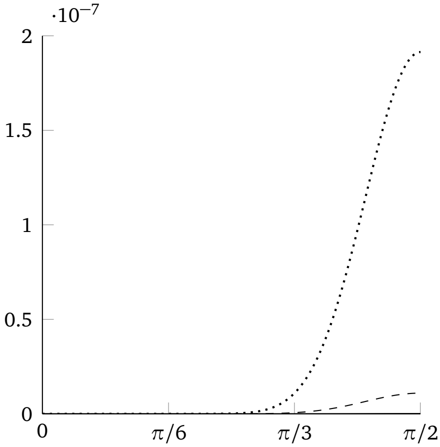
Figure 5.1.: C_R as function of α is plotted for several values of α', for $\ell = 1$ and $\ell = 10$. In all figures we have used $\lambda = 500$nm and $\text{NA} = 0.75$.



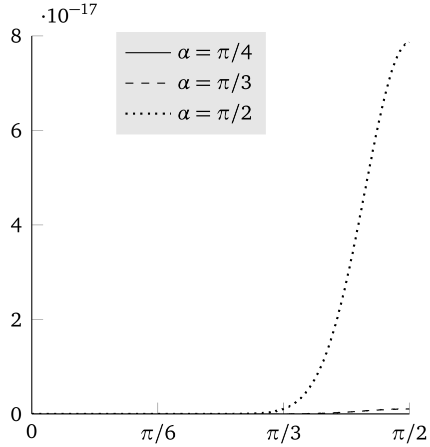
(a) $|S_2 - S_{100}|$ for $R = \lambda/2$ and $\ell = 1$.



(b) $|S_2 - S_{100}|$ for $R = \lambda/2$ and $\ell = 10$.



(c) $|S_{10} - S_{100}|$ for $R = 2\lambda$ and $\ell = 1$.



(d) $|S_{10} - S_{100}|$ for $R = 2\lambda$ and $\ell = 10$.

Figure 5.2.: The absolute errors of C_R as function of α are plotted for several values of α', for $\ell = 1$ and $\ell = 10$. In **(a,b)** the absolute difference between the second and 100th partial sum is given for $R = \lambda/2$. Likewise in **(c,d)** we do the same for $R = 2\lambda$ but we need to compare with the 10th partial sum to get sufficient accuracy. Compare with Figure 5.1 the order of the error. In all figures we have used $\lambda = 500\text{nm}$ and $\text{NA} = 0.75$.

An important case is the case whenever $R \to 0$ as it is possible to give a direct analytical solution. We derive this in Section 5.7.1.

5.5. The optimum fields

5.5.1. The optimum fields in the focal region

The solution to the optimization problem will yield optimal plane wave amplitudes $(A_P, A_S)^{\mathrm{T}}$, but we will also be interested in the electric field in the focal point.

Writing **A** in the Fourier basis, and recalling that we can take real parts gives

$$\mathbf{A}(\alpha,\beta) = \mathrm{Re} \sum_{\ell=-\infty}^{\infty} \mathrm{e}^{i\ell\beta}[\widehat{A}_S(\alpha,\ell)\widehat{\mathbf{s}}(\alpha,\beta) + \widehat{A}_P(\alpha,\ell)\widehat{\mathbf{p}}(\alpha,\beta)], \tag{5.36}$$

Note that that there is only one ℓ in the expansion of the optimum electric field, and that we can take the real part of $(A_P, A_S)^{\mathrm{T}}$, which we will do. Substituting the real part of (5.36) into the expression for the electric field (5.4) we get

$$\mathbf{E}(\mathbf{r}) = \frac{1}{4\pi^2} \sum_{\ell=-\infty}^{\infty} \mathrm{Re} \int_0^{2\pi} \int_0^{\alpha_{\max}} [A_{P,\ell}\mathrm{e}^{i\ell\beta}\widehat{\mathbf{p}} + A_{S,\ell}\mathrm{e}^{i\ell\beta}\widehat{\mathbf{s}}]\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\nu(\alpha)\,\mathrm{d}\beta.$$

The integrals over β can be explicitly computed. Before we proceed with this we will write **r** into cylindrical coordinates. That is

$$\mathbf{r} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \rho\cos\theta \\ \rho\sin\theta \\ z \end{pmatrix}.$$

As we are looking in the focal plane $z = 0$, we can write $\mathbf{k} \cdot \mathbf{r}$ as

$$\mathbf{k} \cdot \mathbf{r} = k \begin{pmatrix} \sin\alpha\cos\beta \\ \sin\alpha\sin\beta \\ \cos\alpha \end{pmatrix} \cdot \begin{pmatrix} \rho\cos\theta \\ \rho\sin\theta \\ 0 \end{pmatrix} = k\rho\sin\alpha\cos(\beta-\theta).$$

Expanding $\widehat{\mathbf{p}}$ and $\widehat{\mathbf{s}}$ we can see that we have to compute integrals of the form

$$\int_0^{2\pi} \psi(\beta)\mathrm{e}^{i\ell\beta}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\,\mathrm{d}\beta,$$

where $\psi(\beta) = 1, \sin\beta$ or $\cos\beta$. These will be named M_ℓ, N_ℓ and O_ℓ respectively. Using the integral representations of the Bessel functions [1, Equation 4.7.6] we find

$$\begin{aligned} M_\ell(\rho,\theta) &:= \int_0^{2\pi} \mathrm{e}^{ik\rho\sin\alpha\cos(\beta-\theta)}\mathrm{e}^{i\ell\beta}\sin\beta\,\mathrm{d}\beta \\ &= \pi i^\ell \mathrm{e}^{i\ell\theta}[\mathrm{e}^{i\theta}J_{\ell+1}(k\rho\sin\alpha) + \mathrm{e}^{-i\theta}J_{\ell-1}(k\rho\sin\alpha)], \\ N_\ell(\rho,\theta) &:= \int_0^{2\pi} \mathrm{e}^{ik\rho\sin\alpha\cos(\beta-\theta)}\mathrm{e}^{i\ell\beta}\cos\beta\,\mathrm{d}\beta \\ &= -\pi i^{\ell-1} \mathrm{e}^{i\ell\theta}[\mathrm{e}^{i\theta}J_{\ell+1}(k\rho\sin\alpha) - \mathrm{e}^{-i\theta}J_{\ell-1}(k\rho\sin\alpha)], \end{aligned}$$

and,

$$\begin{aligned} O_\ell(\rho,\theta) &:= \int_0^{2\pi} \mathrm{e}^{ik\rho\sin\alpha\cos(\beta-\theta)}\mathrm{e}^{i\ell\beta}\,\mathrm{d}\beta \\ &= 2\pi i^\ell \mathrm{e}^{i\ell\theta}J_\ell(k\rho\sin\alpha). \end{aligned}$$

This gives

$$\int_0^{\alpha_{\max}}\int_0^{2\pi} A_P(\alpha,\ell)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathrm{e}^{i\ell\beta}\widehat{\mathbf{p}}(\alpha,\beta)k^2\sin\alpha\cos\alpha\,\mathrm{d}\alpha\,\mathrm{d}\beta$$
$$= \int_0^{\alpha_{\max}} A_P(\alpha,\ell)\begin{pmatrix}-\cos\alpha N_\ell(\rho,\theta)\\ -\cos\alpha M_\ell(\rho,\theta)\\ \sin\alpha O_\ell(\rho,\theta)\end{pmatrix}k^2\sin\alpha\cos\alpha\,\mathrm{d}\alpha.$$

Similarly

$$\int_0^{\alpha_{\max}}\int_0^{2\pi} A_S(\alpha,\ell)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\mathrm{e}^{i\ell\beta}\widehat{\mathbf{s}}(\alpha,\beta)k^2\sin\alpha\cos\alpha\,\mathrm{d}\alpha\,\mathrm{d}\beta$$
$$= \int_0^{\alpha_{\max}} A_S(\alpha,\ell)\begin{pmatrix}M_\ell(\rho,\theta)\\ -N_\ell(\rho,\theta)\\ 0\end{pmatrix}k^2\sin\alpha\cos\alpha\,\mathrm{d}\alpha.$$

We can combine this to obtain

$$\mathbf{E}(\rho,\theta) = \frac{1}{4\pi^2}\sum_{\ell=-\infty}^{\infty}\mathrm{Re}\int_0^{\alpha_{\max}} A_P(\alpha,\ell)\begin{pmatrix}-\cos\alpha N_\ell(\rho,\theta)\\ -\cos\alpha M_\ell(\rho,\theta)\\ \sin\alpha O_\ell(\rho,\theta)\end{pmatrix}\mathrm{d}\nu(\alpha)$$
$$+\frac{1}{4\pi^2}\sum_{\ell=-\infty}^{\infty}\mathrm{Re}\int_0^{\alpha_{\max}} A_S(\alpha,\ell)\begin{pmatrix}-M_\ell(\rho,\theta)\\ N_\ell(\rho,\theta)\\ 0\end{pmatrix}\mathrm{d}\nu(\alpha).$$

5.5.2. The optimum fields in the lens pupil

We compute the optimal fields in the focal point, but we additionally would like to know how to produce these fields. In this section we consider a diffraction limited lens with high numerical aperture, and consider a light beam propagating parallel to the optical axis which is focused by this lens.

Given the plane wave amplitudes **A** of the optimum field in the focal plane of the lens, this optimum can be realized by a proper pupil field in the entrance pupil of the lens. This pupil field can be realized in experiments by using Special Light Modulators (SLMs). The relationship between the pupil field and the plane waves of the focused field is given by the vector diffraction theory of Ignatwkosky [5, 6], Richards and Wolf [9, 12]. This theory is based on two assumptions:

1. The Debye's approximation which allows us to express plane wave amplitudes in image space in the field in the entrance pupil;
2. Abbe's sine condition to guarantee conservation of energy.

In the rest of the section we consider a diffraction limited lens with high numerical aperture NA and a light beam which is focussed by this lens. Next, we consider the standard Euclidean basis $\{\widehat{\mathbf{x}}, \widehat{\mathbf{y}}, \widehat{\mathbf{z}}\}$ in image space such that $\widehat{\mathbf{z}}$ is parallel to the optical axis and where the origin corresponds to the focal point (as is done in our original model). Similarly, let let $\{\widehat{\mathbf{x}}_e, \widehat{\mathbf{y}}_e\}$ be the Euclidean coordinate system in the entrance pupil of the lens such that $\widehat{\mathbf{x}}_e$ and $\widehat{\mathbf{y}}_e$ are parallel to $\widehat{\mathbf{x}}$ and $\widehat{\mathbf{y}}$ respectively. We will use polar coordinates ρ_e and φ_e in the lens pupil.

More explicitly, we write

$$x_e = \rho_e \cos\varphi_e, \quad y_e = \rho_e \sin\varphi_e.$$

The unit vectors $\widehat{\boldsymbol{\rho}}_e$ and $\widehat{\boldsymbol{\varphi}}_e$ are then given by

$$\begin{aligned}
\widehat{\boldsymbol{\rho}}_e &= \cos\varphi_e \widehat{\mathbf{x}}_e + \sin\varphi_e \widehat{\mathbf{y}}_e, \\
\widehat{\boldsymbol{\varphi}}_e &= -\sin\varphi_e \widehat{\mathbf{x}}_e + \cos\varphi_e \widehat{\mathbf{y}}_e.
\end{aligned}$$

Note that $\{\widehat{\boldsymbol{\rho}}_e, \widehat{\boldsymbol{\varphi}}_e, \widehat{\mathbf{z}}\}$ is a positively oriented basis. As the incident beam is predominantly propagating parallel to the optical axis, we neglect the $\widehat{\mathbf{z}}$-component and write electric field at a point (ρ_e, φ_e) of the entrance pupil as

$$\mathbf{E}^e(\rho_e, \varphi_e) = E^e_\rho(\rho_e, \varphi_e)\widehat{\boldsymbol{\rho}}_e + E^p_\varphi(\rho_e, \varphi_e)\widehat{\boldsymbol{\varphi}}_e.$$

The theory of Ignatowsky, Richards and Wolf holds whenever

$$f \gg \frac{\lambda_0}{n\sin^2(\alpha_{\max})}.$$

For a given plane wave of the focused field with wave vector $\mathbf{k} = k_x\widehat{\mathbf{x}} = k_y\widehat{\mathbf{y}} + k_z\widehat{\mathbf{z}}$, we define the corresponding pupil point (x_e, x_e) such that:

$$\begin{aligned} k_x &= -k\frac{kx_e}{f} = -k\frac{\rho_e}{f}\cos\varphi_e, \\ k_y &= -k\frac{ky_e}{f} = -k\frac{\rho_e}{f}\sin\varphi_e. \end{aligned}$$

If we write the vector amplitude $\mathbf{A}$ of the plane wave on the $(\widehat{\mathbf{p}}, \widehat{\mathbf{s}})$ basis as before

$$\mathbf{A}(\mathbf{k}_{||}) = A_S(\mathbf{k}_{||})\widehat{\mathbf{p}}(\widehat{\mathbf{k}}) + A_S(\mathbf{k}_{||})\widehat{\mathbf{s}}(\widehat{\mathbf{k}}).$$

Then in the theory of Ignatowsky, Richards and Wolf, the radial component of the pupil field is related to the P-component of the electric field of the plane wave, whereas the azimuthal component of the pupil field is related to the S-component of the field of the plane wave. In fact, there holds:

$$E^e_\rho(\rho_e, \varphi_e) = \frac{\sqrt{kk_z}}{2\pi i f}A_P\Big(-k\frac{\rho_e}{f}\cos\varphi_e, -k\frac{\rho_e}{f}\sin\varphi_e\Big) \tag{5.37}$$

$$E^e_\varphi(\rho_e, \varphi_e) = \frac{\sqrt{kk_z}}{2\pi i f}A_S\Big(-k\frac{\rho_e}{f}\cos\varphi_e, -k\frac{\rho_e}{f}\sin\varphi_e\Big), \tag{5.38}$$

where the factor $\sqrt{kk_z}$ is included to account for energy conservation and where

$$k_z = k\sqrt{1 - \frac{\rho_e^2}{f^2}}$$

Hence, $\mathbf{E}^e$ becomes

$$\begin{aligned}\mathbf{E}^e(\rho_e, \varphi_e) = &\frac{\sqrt{kk_z}}{2\pi i f}\Big\{A_P(-k_x, -k_y)\cos\varphi_e - A_S(-k_x, -k_y)\sin\varphi_e\Big\}\widehat{\mathbf{x}} \\ &+ \frac{\sqrt{kk_z}}{2\pi i f}\Big\{A_P(-k_x, -k_y)\sin\varphi_e + A_S(-k_x, -k_y)\cos\varphi_e\Big\}\widehat{\mathbf{y}}.\end{aligned}$$

The $\mathbf{A}$ we obtain is given in terms of the angles α and β. For α we see that $f\sin\alpha = \rho_e$ where f is the focal length. Whereas angle β corresponds to the $\varphi_e + \pi$ to incorporate for the minus sign in (x_e, y_e) in the lens pupil. Concluding that

$$\alpha = \arcsin\Big(\frac{1}{k}\sqrt{k_x^2 + k_y^2}\Big), \quad \sin\beta = -\frac{k_x}{|\mathbf{k}_{||}|} \quad \text{and, } \cos\beta = -\frac{k_y}{|\mathbf{k}_{||}|}.$$

Polarization

In this section we derive expressions for the polarization.

Recall (5.1). For the general electric field in the entrance pupil of the lens $\mathscr{E}(\mathbf{r}, t)$ we can write

$$\mathscr{E}^e(\mathbf{r}, t) = \text{Re}[\mathbf{E}^e(\mathbf{r}, t)\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}].$$

As $\mathbf{A}$ is real, and noting that $\text{Re}(-i\mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}) = \sin(\mathbf{k}\cdot\mathbf{r} - \omega t)$ we get

$$\begin{aligned}\mathscr{E}^e(\mathbf{r}, t) := &\frac{\sqrt{kk_z}}{2\pi f}\sin(\mathbf{k}\cdot\mathbf{r} - \omega t) \\ &\times \begin{pmatrix} A_P(-k_x, -k_y)\cos\varphi - A_S(-k_x, -k_y)\sin\varphi \\ A_P(-k_x, -k_y)\sin\varphi + A_S(-k_x, -k_y)\cos\varphi \end{pmatrix}.\end{aligned}$$

As the solution to the integral equation for general $R > 0$ will not be directly computable, we will proceed numerically in this case. Afterwards we will show how to solve the case for $R = 0$ analytically.

5.6. Discretization of the integral equation

In this section we will discretize (5.33). For brevity we will for each $\ell \in \mathbb{Z}$ discretize

$$\Lambda \begin{pmatrix} \widehat{A}_P(\alpha,\ell) \\ \widehat{A}_S(\alpha,\ell) \end{pmatrix} = \int_0^{\alpha_{\max}} \widehat{\mathbf{M}}_R(\alpha,\alpha',\ell) \begin{pmatrix} \widehat{A}_P(\alpha',\ell) \\ \widehat{A}_S(\alpha',\ell) \end{pmatrix} k^2 \sin\alpha' \cos\alpha' \,\mathrm{d}\alpha' \quad (5.39)$$

into a matrix equation. As a first step we will discretize the integral. For convenience, we subtitute $s : \alpha \to (\alpha+1)\alpha_{\max}/2$ to obtain

$$\Lambda \begin{pmatrix} \widehat{A}_P(s(\alpha),\ell) \\ \widehat{A}_S(s(\alpha),\ell) \end{pmatrix} = \frac{\alpha_{\max}}{2} \int_{-1}^{1} \widehat{\mathbf{M}}'_R(s(\alpha),s(\alpha'),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha'),\ell) \\ \widehat{A}_S(s(\alpha'),\ell) \end{pmatrix} \mathrm{d}\alpha' \quad (5.40)$$

where we have set

$$\widehat{\mathbf{M}}'_R(s(\alpha),s(\alpha'),\ell) := k^2 \widehat{\mathbf{M}}_R(s(\alpha),s(\alpha'),\ell) \sin(s(\alpha')) \cos(s(\alpha')).$$

We will discretize the integral with the Gaussian quadrature rule on that interval, which will, given the number of data points N return node points $-1 = \alpha'_1 < \alpha'_2 < \ldots < \alpha'_N = 1$ and weights $(w_n)_{n=1}^N$ so that we can write

$$\Lambda \begin{pmatrix} \widehat{A}_P(s(\alpha),\ell) \\ \widehat{A}_S(s(\alpha),\ell) \end{pmatrix} = \frac{\alpha_{\max}}{2} \sum_{n=1}^{N} w_n \widehat{\mathbf{M}}'_R(s(\alpha),s(\alpha'_n),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha'_n),\ell) \\ \widehat{A}_S(s(\alpha'_n),\ell) \end{pmatrix}.$$

If we discretize α on the integration node points, we get a collection of m equations, that is for each $m = 1,\ldots,N$ we have

$$\Lambda \begin{pmatrix} \widehat{A}_P(s(\alpha_m),\ell) \\ \widehat{A}_S(s(\alpha_m),\ell) \end{pmatrix} = \frac{\alpha_{\max}}{2} \sum_{n=1}^{N} w_n \widehat{\mathbf{M}}'_R(s(\alpha_m),s(\alpha'_n),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha'_n),\ell) \\ \widehat{A}_S(s(\alpha'_n),\ell) \end{pmatrix}.$$

We will rewrite this into a classical matrix eigenvalue problem. To see how this works we pick $N = 2$ and obtain the two equations

$$\Lambda \begin{pmatrix} \widehat{A}_P(s(\alpha_1),\ell) \\ \widehat{A}_S(s(\alpha_1),\ell) \end{pmatrix} = \frac{\alpha_{\max}}{2} w_1 \widehat{\mathbf{M}}_R'(s(\alpha_1), s(\alpha_1'),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha_1'),\ell) \\ \widehat{A}_S(s(\alpha_1'),\ell) \end{pmatrix} + \frac{\alpha_{\max}}{2} w_2 \widehat{\mathbf{M}}_R'(s(\alpha_1), s(\alpha_2'),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha_2'),\ell) \\ \widehat{A}_S(s(\alpha_2'),\ell) \end{pmatrix},$$

and,

$$\Lambda \begin{pmatrix} \widehat{A}_P(s(\alpha_2),\ell) \\ \widehat{A}_S(s(\alpha_2),\ell) \end{pmatrix} = \frac{\alpha_{\max}}{2} w_1 \widehat{\mathbf{M}}_R'(s(\alpha_2), s(\alpha_1'),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha_1'),\ell) \\ \widehat{A}_S(s(\alpha_1'),\ell) \end{pmatrix} + \frac{\alpha_{\max}}{2} w_2 \widehat{\mathbf{M}}_R'(s(\alpha_2), s(\alpha_2'),\ell) \begin{pmatrix} \widehat{A}_P(s(\alpha_2'),\ell) \\ \widehat{A}_S(s(\alpha_2'),\ell) \end{pmatrix}.$$

We set $\mathbf{w} = \mathrm{diag}\{w_1, w_2\}$ and let $\mathbf{W} = \mathrm{diag}\{\mathbf{w}, \mathbf{w}\}$. Next we define the block matrix $\mathbf{M}_D$

$$\mathbf{M}_D := \begin{pmatrix} \mathbf{M}_D^{11} & \mathbf{M}_D^{12} \\ \mathbf{M}_D^{21} & \mathbf{M}_D^{22} \end{pmatrix}, \tag{5.41}$$

where the matrices $\mathbf{M}_D^{mn}$ as

$$\mathbf{M}_D^{mn} := \begin{pmatrix} \widehat{M}_{R,mn}'(s(\alpha_1), s(\alpha_1')) & \widehat{M}_{R,mn}'(s(\alpha_1), s(\alpha_2')) \\ \widehat{M}_{R,mn}'(s(\alpha_2), s(\alpha_1')) & \widehat{M}_{R,mn}'(s(\alpha_2), s(\alpha_2')) \end{pmatrix}.$$

So, we can rewrite (5.6, 5.6) as the classical eigenvalue problem

$$\frac{2\Lambda}{\alpha_{\max}} \begin{pmatrix} \widehat{A}_P(s(\alpha_1),\ell) \\ \widehat{A}_P(s(\alpha_2),\ell) \\ \widehat{A}_S(s(\alpha_1),\ell) \\ \widehat{A}_S(s(\alpha_2),\ell) \end{pmatrix} = \mathbf{M}_D \mathbf{W} \begin{pmatrix} \widehat{A}_P(s(\alpha_1),\ell) \\ \widehat{A}_P(s(\alpha_2),\ell) \\ \widehat{A}_S(s(\alpha_1),\ell) \\ \widehat{A}_S(s(\alpha_2),\ell) \end{pmatrix},$$

We can easily generalize this to N datapoints. Start by letting $(\alpha_i)_{i=1}^N$ be the integration nodes with corresponding weights $(w_i)_{i=1}^N$ and set

$$\boldsymbol{\alpha} := \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix}, \mathbf{w} = \operatorname{diag}\{w_1, \ldots, w_N\} \text{ and } \mathbf{W} = \operatorname{diag}\{\mathbf{w}, \mathbf{w}\}.$$

The matrices $\mathbf{M}_D^{mn}$ in $\mathbf{M}_D$ as given in (5.41) for the general case are defined by

$$\mathbf{M}_D^{mn} := \widehat{M}'_{R,mn}(s(\boldsymbol{\alpha}), s(\boldsymbol{\alpha}')).$$

Using this, we can write the discretized equation as an eigenvalue problem

$$\frac{2\Lambda}{\alpha_{\max}} \begin{pmatrix} \widehat{A}_P(s(\boldsymbol{\alpha}), \ell) \\ \widehat{A}_S(s(\boldsymbol{\alpha}), \ell) \end{pmatrix} = \mathbf{M}_D \mathbf{W} \begin{pmatrix} \widehat{A}_P(s(\boldsymbol{\alpha}), \ell) \\ \widehat{A}_S(s(\boldsymbol{\alpha}), \ell) \end{pmatrix}. \tag{5.42}$$

As we discretized a homogeneous Fredholm equation of the second kind, we obtained a classical eigenvalue problem, hence we have consider the numerical stability.

5.6.1. Numerical stability

The method we have used above is also refered to as the Nyström method. For our discretized problem to approximate our original problem we need to have that the solution (5.42) converges to the solution of the integral equation (5.39) whenever we send N to infinity.

As we have seen in Section 5.4 on the mathematical properties of the solution we have noted that the operator we study is compact. Hence we can apply [10, Theorem 3]. The only difficulty that can arise from applying the theorem it is stated for scalar kernels while we have a matrix-valued kernel.

We can reduce our vector-valued problem to a scalar valued one. Consider (5.40) and set

$$K_\ell(\alpha,\alpha') = \begin{cases} \widehat{M}'_{R,11}(s(\alpha+1), s(\alpha'+1), \ell) & \text{if } (\alpha,\alpha') \in (-2,0)\times(-2,0), \\ \widehat{M}'_{R,12}(s(\alpha+1), s(\alpha'-1), \ell) & \text{if } (\alpha,\alpha') \in (-2,0)\times(0,2), \\ \widehat{M}'_{R,21}(s(\alpha-1), s(\alpha'+1), \ell) & \text{if } (\alpha,\alpha') \in (0,2)\times(-2,0), \\ \widehat{M}'_{R,22}(s(\alpha-1), s(\alpha'-1), \ell) & \text{if } (\alpha,\alpha') \in (0,2)\times(0,2). \end{cases}$$

Using this scalar kernel, we can formulate the scalar-valued Fredhom problem

$$\Lambda A_\ell(\alpha) = \frac{\alpha_{\max}}{2}\int_{-2}^{2} K_\ell(\alpha,\alpha') A_\ell(\alpha')\,\mathrm{d}\alpha', \tag{5.43}$$

and note that we can recover $\widehat{A}_P$ and $\widehat{A}_S$ through

$$A_\ell(\alpha) = \begin{cases} \widehat{A}_P(s(\alpha+1,\ell) & \text{if } \alpha \in (-2,0), \\ \widehat{A}_S(s(\alpha-1),\ell) & \text{if } \alpha \in (0,2). \end{cases}$$

Discretizing (5.43) yields the same discretization as (5.42) and in this form we can apply [10, Theorem 3] to obtain numerical stability for our original problem (5.42).

Remark: expansion into polynomials Instead of using discretizing the equation directly, would could note that

$$\langle p, q\rangle = k^2 \int_0^{\alpha_{\max}} p(\sin\alpha) q(\sin\alpha) \sin\alpha\cos\alpha\,\mathrm{d}\alpha,$$

defines an inner product as $\sin\alpha\cos\alpha\,\mathrm{d}\alpha$ is a positive measure on $[0,\alpha_{\max}]$. Using this we can apply the Gram-Schmidt algorithm to get a polynomial basis in $\sin\alpha$ for the L^2 space with respect to this measure. Using this basis we can expand the equation over α into a basis just as we have done with the Fourier basis over β.

5.7. The solution

In this section we compute the solution to (5.34) for the optimal ℓ. First we will solve the case $R \to 0$ which can be done analytically and for the case for general $R > 0$ we provide a numerical scheme and the solutions thereof.

5.7.1. The case $R \to 0$

In this section we compute the solution for $R \to 0$ analytically. As a first step we consider what happens with the functional F in (5.8) when $R \to 0$. Through the Lebesgue Differentiation Theorem [3, Theorem 3.21] we can see that

$$\lim_{R\to 0} F(\mathbf{A}, R) = |\mathbf{E}(\mathbf{0})|^2.$$

So, the case $R \to 0$ optimizes the electric energy density in the focal point. To see what our model in (5.19) reduces to we need to compute C_R as $R \to 0$. Considering the series expansion (5.10) we see that $C_R \to \frac{1}{4\pi^2}$ as $R \to 0$. So, we can write (5.12) as:

$$F(\mathbf{A}, 0, z) := \langle \mathbf{A} * C_0, \mathbf{A} \rangle_{L^2(\Omega)}.$$

From (5.19) we deduced that for the case $R \to 0$ the optimal $\mathbf{A}$ should satisfy

$$\Lambda \mathbf{A} = \frac{1 * \mathbf{A}}{k_z} \text{ in } \Omega.$$

As in the general case (5.34), we need to compute the Fourier coefficients of $\mathbf{M}_0(\alpha, \alpha', \cdot) * \mathbf{A}(\alpha', \cdot)$ in β. The fact that $C_0 = \frac{1}{4\pi^2}$ in turn implies that

$\widehat{C}_0(\ell) = \frac{\delta_{\ell,0}}{4\pi^2}$. Hence, again using (5.35) we can see that $\widehat{\mathbf{M}}_0$ is given by:

$$\begin{aligned}
\widehat{\mathbf{M}}_0(\alpha,\alpha',\ell) &= \frac{1}{4\pi^2}\frac{1}{k\cos\alpha}\widehat{\mathbf{M}}(\alpha,\alpha',\ell) \\
&= \frac{1}{4\pi^2}\delta_{\ell,0}\frac{1}{k\cos\alpha}\begin{pmatrix}\sin\alpha\sin\alpha' & 0 \\ 0 & 0\end{pmatrix} \\
&\quad + \frac{1}{4\pi^2}\frac{\delta_{\ell,\pm 1}}{2}\frac{1}{k\cos\alpha}\begin{pmatrix}\cos\alpha\cos\alpha' & \pm i\cos\alpha \\ \mp i\cos\alpha' & 1\end{pmatrix}.
\end{aligned}$$

Set $\Lambda' = 4\pi^2\Lambda$, then by (5.34) we need to solve

$$\Lambda'\begin{pmatrix}\widehat{A}_P(\alpha,\ell) \\ \widehat{A}_S(\alpha,\ell)\end{pmatrix} = \int_0^{\alpha_{\max}} \frac{1}{k\cos\alpha}\widehat{\mathbf{M}}(\alpha,\alpha',\ell)\begin{pmatrix}\widehat{A}_P(\alpha',\ell) \\ \widehat{A}_S(\alpha',\ell)\end{pmatrix} \mathrm{d}\nu(\alpha'). \qquad (5.44)$$

There are three non-zero cases for ℓ. Namely $\ell = 0$ and $\ell = \pm 1$. Since we have shown before that it is sufficient to consider nonnegative ℓ, we only look at $\ell = 0$ and $\ell = 1$. Starting with $\ell = 0$ we immediately get from (5.44) that $\widehat{A}_S(\alpha, 0) = 0$. While for $\widehat{A}_P$ we need to solve the equation

$$\Lambda\widehat{A}_P(\alpha,0) = k\int_0^{\alpha_{\max}} \frac{1}{\cos\alpha}\sin\alpha\sin\alpha'\widehat{A}_P(\alpha,0)\sin\alpha'\cos\alpha'\,\mathrm{d}\alpha'.$$

Implying that $\widehat{A}_P(\alpha,0)$ is proportional to $\tan\alpha$. Substituting this for the eigenvalue in (5.44) yields

$$\Lambda_0' = k\int_0^{\alpha_{\max}} \sin^3\alpha'\,\mathrm{d}\alpha' = \frac{k}{3}[\cos(\alpha_{\max})^3 - 3\cos(\alpha_{\max}) + 2]. \qquad (5.45)$$

For $\ell = 1$ we can expand (5.44) to see that $\widehat{A}_P$ should be of the form $\widehat{A}_P = \xi_P$ and $\widehat{A}_S = \xi_S\frac{1}{\cos\alpha}$ for some constants ξ_S and ξ_P. By substituting these again into (5.44) we obtain

$$\begin{aligned}
\Lambda'\xi_P &= \frac{k}{2}\int_0^{\alpha_{\max}}\Big(\cos\alpha'\xi_P + i\xi_S\frac{1}{\cos\alpha'}\Big)\sin\alpha'\cos\alpha'\,\mathrm{d}\alpha' \\
&= \xi_P\frac{k}{2}\int_0^{\alpha_{\max}}\cos^2\alpha'\sin\alpha'\,\mathrm{d}\alpha' + i\xi_S\frac{k}{2}\int_0^{\alpha_{\max}}\sin\alpha'\,\mathrm{d}\alpha' \\
&= \xi_P I_1 + i\xi_S I_2.
\end{aligned}$$

And,

$$\begin{aligned}
\Lambda'\xi_S &= \frac{k}{2}\int_0^{\alpha_{\max}}\Big(-\xi_P i\cos\alpha' + \xi_S\frac{1}{\cos\alpha'}\Big)\sin\alpha'\cos\alpha'\,\mathrm{d}\alpha' \\
&= -\xi_P i\frac{k}{2}\int_0^{\alpha_{\max}}\sin\alpha'\cos^2\alpha'\,\mathrm{d}\alpha' + \xi_S\frac{k}{2}\int_0^{\alpha_{\max}}\sin\alpha'\,\mathrm{d}\alpha' \\
&= -\xi_P i I_1 + \xi_S I_2.
\end{aligned}$$

Where we have defined I_1, I_2 as:

$$\begin{aligned}
I_1 &:= \frac{k}{2}\int_0^{\alpha_{\max}}\sin\alpha'\cos^2\alpha'\,\mathrm{d}\alpha' = \frac{k}{6}(1-\cos^3\alpha_{\max}), \\
I_2 &:= \frac{k}{2}\int_0^{\alpha_{\max}}\sin\alpha'\,\mathrm{d}\alpha' = \frac{k}{2}(1-\cos\alpha_{\max}).
\end{aligned}$$

Summarizing, this gives us the system:

$$\Lambda'\begin{pmatrix}\xi_P\\ \xi_S\end{pmatrix} = \begin{pmatrix} I_1 & iI_2 \\ -iI_1 & I_2\end{pmatrix}\begin{pmatrix}\xi_P\\ \xi_S\end{pmatrix}.$$

The largest eigenvalue of this system is $I_1 + I_2$, and we can see that for all $\alpha_{\max}$ this is always larger than eigenvalue (5.45) corresponding to $\ell = 0$. The eigenvector corresponding to this eigenvalue $I_1 + I_2$ is

$$\begin{pmatrix}\xi_P\\ \xi_S\end{pmatrix} = \begin{pmatrix} i\\ 1\end{pmatrix}.$$

So, the solution is given by:

$$A_P(\alpha,\beta) = i\mathrm{e}^{i\beta},$$
$$A_S(\alpha,\beta) = \frac{\mathrm{e}^{i\beta}}{\cos\alpha}.$$

As we have seen before, there is always a real solution by taking real parts. For our case this gives

$$A_P(\alpha,\beta) = \mathrm{Re}\{i\mathrm{e}^{i\beta}\} = -\sin\beta,$$
$$A_S(\alpha,\beta) = \mathrm{Re}\left\{\frac{\mathrm{e}^{i\beta}}{\cos\alpha}\right\} = \frac{\cos\beta}{\cos\alpha}.$$

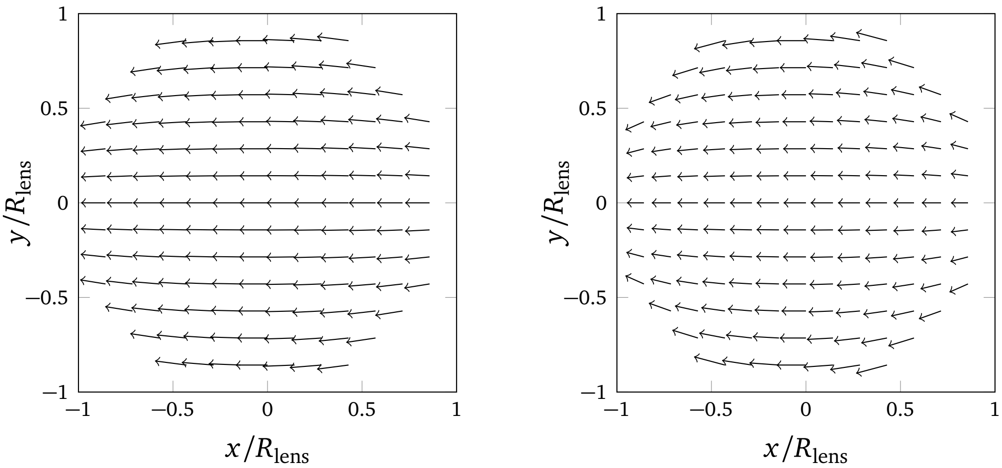
We can compute the field in the lens pupil using Section 5.5. Recall that $\mathbf{A}(\alpha,\beta)$ is a shorthand for $\mathbf{A}(k\sin\alpha\cos\beta, k\sin\alpha\sin\beta)$ and that $f\sin\alpha = \rho_p$. Combining the results from Section 5.5.2 with $\cos\alpha = \sqrt{1-\frac{\rho_p^2}{f^2}}$ gives us

$$\mathbf{E}^e_\rho(\rho_e,\varphi_e) = \frac{\sqrt{kk_z}}{2\pi i f}A_P\Big(k\frac{\rho_p}{f}\cos\varphi, k\frac{\rho_p}{f}\sin\varphi\Big) = -\frac{k\sin\varphi}{2\pi i f}\frac{(f^2-\rho^2)^{1/4}}{\sqrt{f}},$$
$$\mathbf{E}^e_\varphi(\rho_e,\varphi_e) = \frac{\sqrt{kk_z}}{2\pi i f}A_S\Big(k\frac{\rho_p}{f}\cos\varphi, k\frac{\rho_p}{f}\sin\varphi\Big) = \frac{k\cos\varphi}{2\pi i f}\frac{\sqrt{f}}{(f^2-\rho^2)^{1/4}}.$$

To incorporate the mirror image $(k_x,k_y)\to(-k_x,-k_y)$ we set $\beta\to\varphi_e+\pi$ in (5.37) and (5.38) and we can plot the pupil field, show in Figure 5.3 for $\mathrm{NA}=0.75$ and $\mathrm{NA}=0.95$. We see that in both cases the field is linearly polarized for $R=0$, which is consistent with the results in [2].

5.7.2. The case for general $R>0$

This case for $R>0$ is difficult to solve analyically, and even if it were possible it is unlikely that it would yield more information than the numerical solution as sketched in Section 5.6.



(a) NA $= 0.75$ **(b)** NA $= 0.95$

Figure 5.3.: The entrance pupil field (E_x^e, E_y^p) for the case $R \to 0$.

5.8. Results

5.8.1. Which NA and R give the highest energy density?

If we wish to plot F_{opt} with respect to NA and R the first thing we have to do is select the ℓ which gives for a fixed NA and fixed R the largest F_{opt}. This is implemented in the code to generate the images below. First we loop over ℓ and store all maximal energies F_{opt} and then select the ℓ corresponding to the maximal one. If we fix R we get the following numerical values for NA which give us for the optimal $\ell = 0$, and in all other cases $\ell = 1$:

1. $R = \lambda/2$ all values of NA give optimal $\ell = 1$.

2. $R = \lambda$ for NA in $[0.77\lambda, 0.90\lambda]$ we have $\ell = 0$, else $\ell = 1$.

3. $R = 2\lambda$ for NA in $[0.46\lambda, 0.56\lambda] \cup [0.68\lambda, 0.76\lambda] \cup [0.88\lambda, 0.94\lambda]$

we have $\ell = 0$, else $\ell = 1$.

Similarly, if we fix NA and vary R we get

1. for $NA = 0.75$, we have $\ell = 0$ for R in $[\lambda, 1.35\lambda] \cup [1.75\lambda, 2\lambda]$ otherwise $\ell = 1$.

2. for $NA = 0.95]$, we have $\ell = 0$ for R in $[0.7\lambda, 0.9\lambda] \cup [1.25\lambda, 1.45\lambda] \cup [1.8\lambda, 2\lambda]$ otherwise $\ell = 1$.

5.8.2. The normalized distribution $|E_x|^2$, $|E_y|^2$, $|E_z|^2$ and $|\mathbf{E}|^2$ in the focal point

In this section we use the numerical method from Section 5.6 to compute the cross-sections for $x = 0$ of the components of $|\mathbf{E}|^2$. We do this in the cases $R = 0, \lambda/2$ and 2λ. This result is given in Figure 5.4. We also plot the complete fields for $R = 0$ and $R = 2\lambda$ in Figures 5.6 and 5.5 respectively.

5.9. The field in the lens pupil

Using the results from Section 5.5.2 we can plot the fields in the entrance pupil of the lens. We do this for NA $= 0.75$ and $R = \lambda/2, \lambda$ and 2λ.

5.10. A bit of mathematics

5.10.1. The Fourier transform

In this section we briefly summarize some results concerning the Fourier transform. For the Fourier transform several normalizations are known,

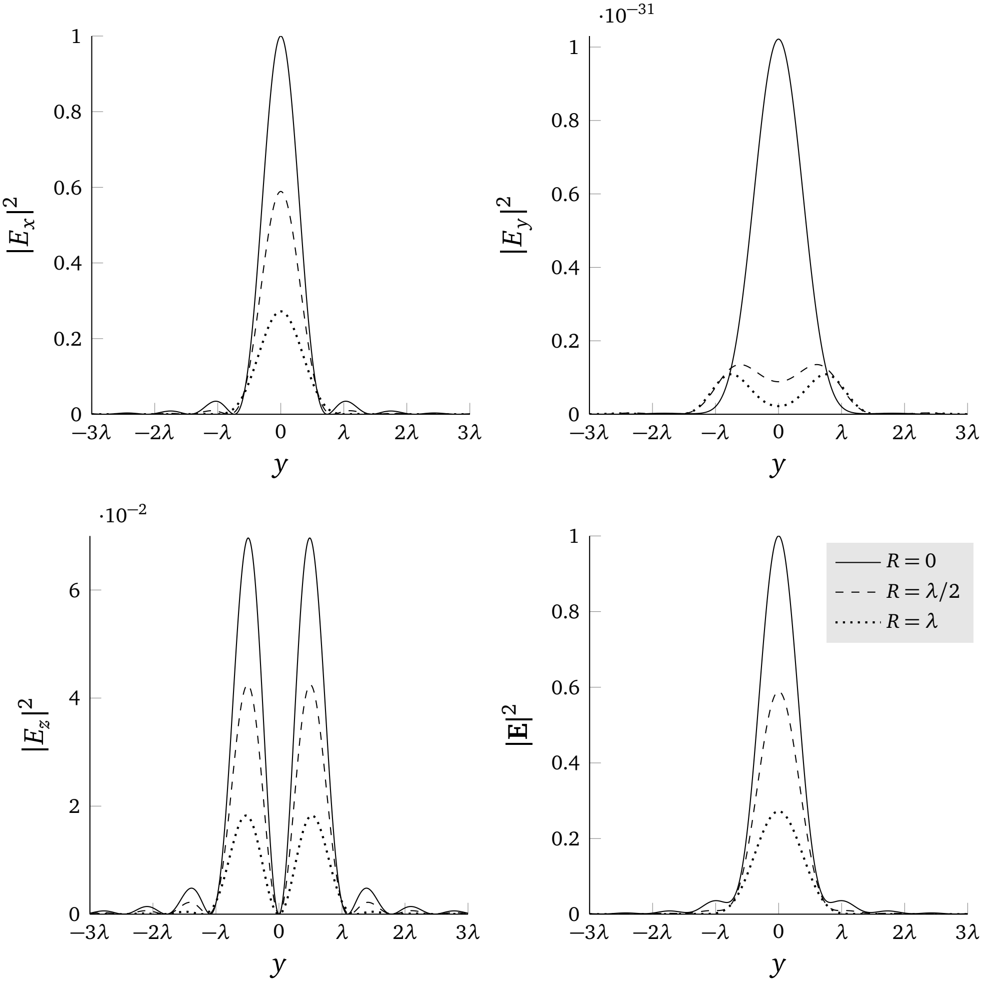
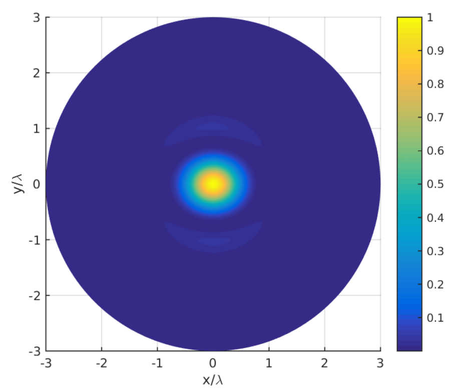
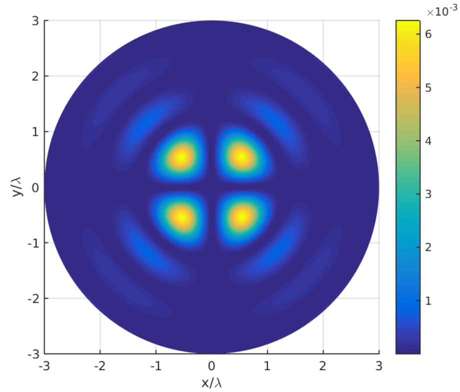


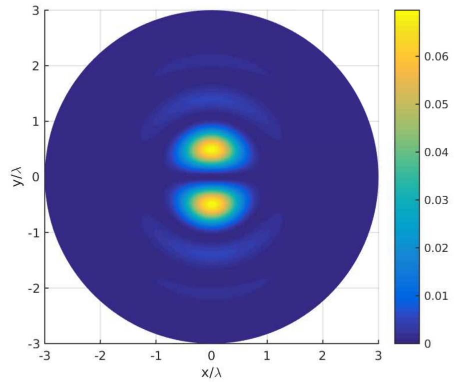
Figure 5.4.: The amplitudes of the components of $\mathbf{E}(x = 0)$ are given for NA = 0.75, $\lambda = 500$nm and $R = 0, \lambda/2$ and λ. These are normalized against the maximum of $|\mathbf{E}|^2$ for $R = 0$. In each case $\ell = 1$ is the optimal coefficient.



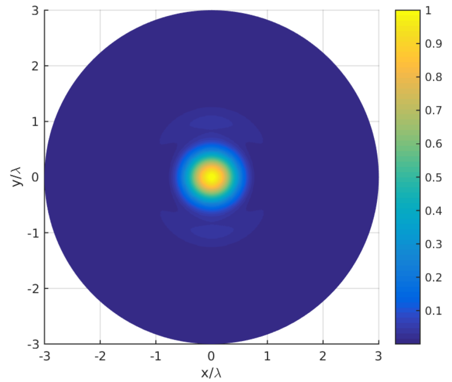
(a) $|E_x|^2$



(b) $|E_y|^2$

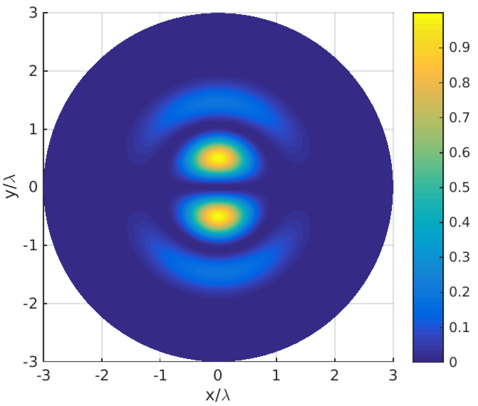


(c) $|E_z|^2$

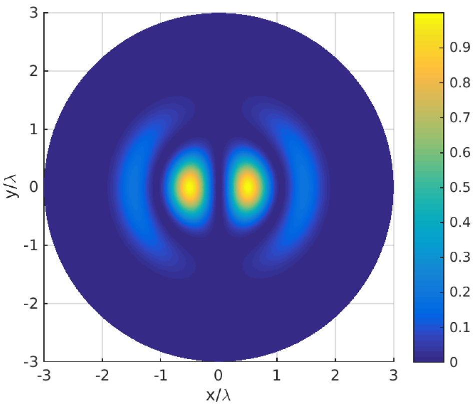


(d) $|\mathbf{E}|^2$

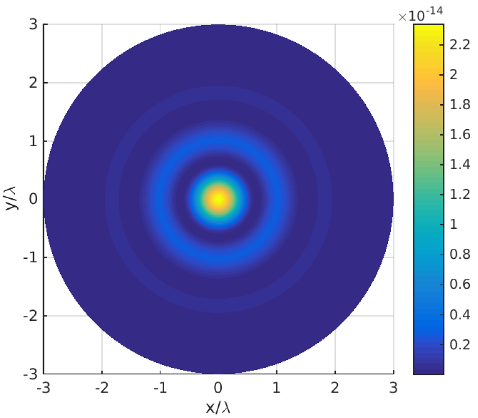
Figure 5.5.: The amplitudes of the components of **E** are given for NA $= 0.75$, $\lambda = 500$nm in the case $R = 0$. These are normalized against the maximum of $|\mathbf{E}|^2$. $\ell = 1$ is the optimal coefficient.



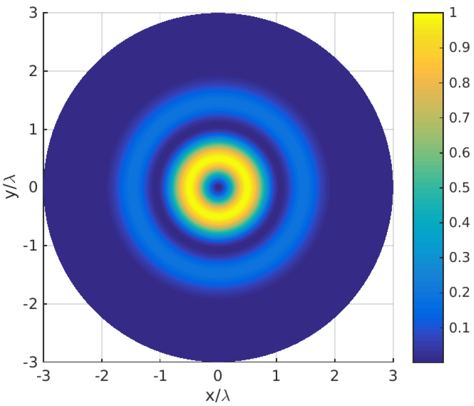
(a) $|E_x|^2$



(b) $|E_y|^2$

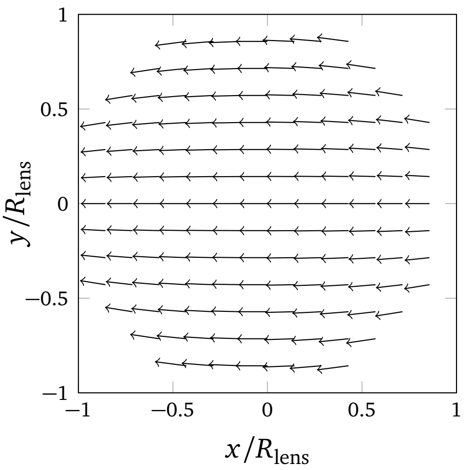


(c) $|E_z|^2$

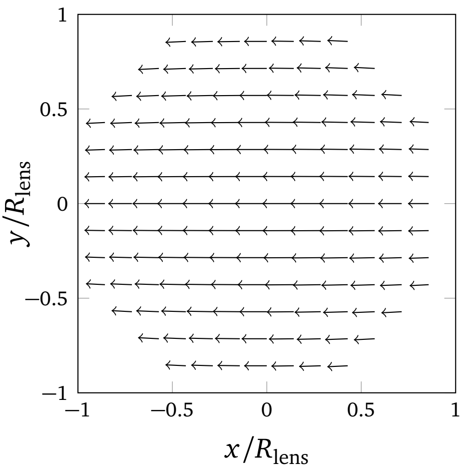


(d) $|\mathbf{E}|^2$

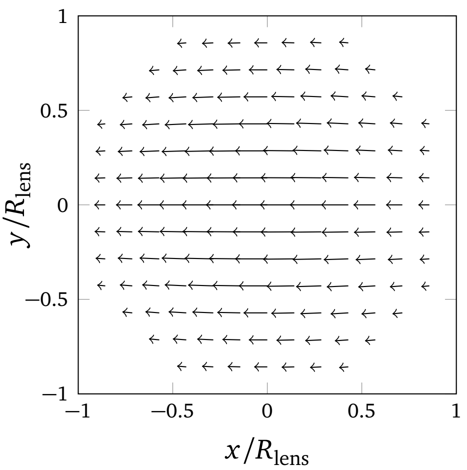
Figure 5.6.: The amplitudes of the components of **E** are given for NA $= 0.75$, $\lambda = 500$nm in the case $R = 2\lambda$. These are normalized against the maximum $|\mathbf{E}|^2$. $\ell = 0$ is the optimal coefficient.



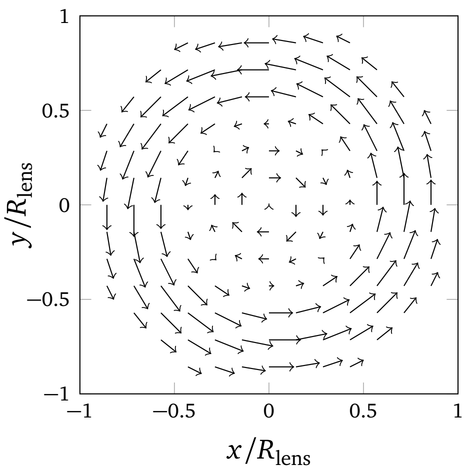
(a) $R = 0$



(b) $R = \lambda/2$



(c) $R = \lambda$



(d) $R = 2\lambda$

Figure 5.7.: The vector field (E_x^p, E_y^p) in the pupil is shown for $R = 0, \lambda$ and 2λ. For the cases $R = 0, \lambda/2$ and λ the pupil field is linearily polarized, whereas for the case $R = 2\lambda$ gives a azimuthal polarized optimum.

and define the Fourier transform of **A** in Euclidean coordinates pointwise as [4, Definition 5.7]

$$\begin{aligned}\mathscr{F}(\mathbf{A})(k_x,k_y) &= \iint_{\mathbf{R}^2} \mathbf{A}(k'_x,k'_y)\mathrm{e}^{-i(k'_x k_x + k'_y k_y)}\,\mathrm{d}\mathbf{k}'_{\|} \\ &= \iint_{\mathbf{R}^2} \mathbf{A}(\mathbf{k}'_{\|})\mathrm{e}^{-i\mathbf{k}'_{\|}\cdot\mathbf{k}_{\|}}\,\mathrm{d}\mathbf{k}'_{\|}\end{aligned} \tag{5.46}$$

with inverse

$$\mathscr{F}^{-1}(\mathbf{A})(k_x,k_y) = \frac{1}{4\pi^2}\iint_{\mathbf{R}^2} \mathbf{A}(\mathbf{k}'_{\|})\mathrm{e}^{i\mathbf{k}'_{\|}\cdot\mathbf{k}_{\|}}\,\mathrm{d}\mathbf{k}'_{\|} \tag{5.47}$$

So that we have the convolution identity [4, Theorem 5.6]:

$$\mathscr{F}(AB)(\mathbf{k}_{\|}) = (\mathscr{F}(A) * \mathscr{F}(B)(\mathbf{k}_{\|}) = \iint_{\mathbf{R}^2} A(\mathbf{k}_{\|} - \mathbf{k}'_{\|})B(\mathbf{k}'_{\|})\,\mathrm{d}\mathbf{k}'_{\|} \tag{5.48}$$

While Parseval's formula is [4, Theorem 5.5]

$$\langle A,B\rangle_{L^2(\mathbf{R}^2)} = \frac{1}{4\pi^2}\langle \mathscr{F}(A), \mathscr{F}(B)\rangle_{L^2(\mathbf{R}^2)}. \tag{5.49}$$

5.11. The Fourier coefficients of C_R

In this section we compute the Fourier coefficients of C_R which are used in the main text in the definition of $\mathbf{M}_R$. As a first step, we expand the Bessel function J_1 of (5.10) into its Taylor series.

$$C_R(|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|) = \frac{1}{2\pi^2}\frac{J_1(R|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|)}{R|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|} = \frac{1}{4\pi^2}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!(k+1)!}\left(\frac{R|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|}{2}\right)^{2k}. \tag{5.50}$$

As a next step, we set $x = |\mathbf{k}_{\|} - \mathbf{k}'_{\|}|$ and recall (5.27) to which we apply the binomial theorem after setting $\beta - \beta' =: \gamma$:

$$(\sin^2\alpha + \sin^2\alpha' - 2\sin\alpha\sin\alpha'\cos\gamma)^k$$
$$= \sum_{\ell=0}^{k} \binom{k}{\ell} (-1)^\ell \cos^\ell\gamma (2\sin\alpha\sin\alpha')^\ell (\sin^2\alpha + \sin^2\alpha')^{k-\ell}$$

Combining with (5.50):

$$C_R(|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|) = \frac{1}{4\pi^2} \sum_{\ell=0}^{\infty} \sum_{m=\ell}^{\infty} \frac{(-1)^{m+\ell}}{(m+1)!\ell!(m-\ell)!}$$
$$\times \left(\frac{Rk}{2}\right)^{2m} \cos^\ell\gamma (2\sin\alpha\sin\alpha')^\ell (\sin^2\alpha + \sin^2\alpha')^{m-\ell}.$$

In the next step, we apply the binomial theorem to $2\cos\gamma = \mathrm{e}^{i\gamma} + \mathrm{e}^{-i\gamma}$. Combining and rearranging gives

$$C_R(|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|) = \frac{1}{4\pi^2} \sum_{\ell=0}^{\infty} \mathrm{e}^{i\ell\gamma} \sum_{s=0}^{\ell} \binom{\ell}{s} \mathrm{e}^{-2is\gamma} (\sin\alpha\sin\alpha')^\ell$$
$$\times \sum_{m=\ell}^{\infty} \frac{(-1)^{m+\ell}}{(m+1)!\ell!(m-\ell)!} \left(\frac{Rk}{2}\right)^{2m} (\sin^2\alpha + \sin^2\alpha')^{m-\ell}.$$

Rearranging the sums gives

$$C_R(|\mathbf{k}_{\|} - \mathbf{k}'_{\|}|) = \frac{1}{4\pi^2} \sum_{\ell=-\infty}^{\infty} \mathrm{e}^{i\ell\gamma} \sum_{s=\max(0,-\ell)}^{\infty}$$
$$\times \sum_{m=0}^{\infty} \frac{(-1)^m (\sin\alpha\sin\alpha')^{\ell+2s}}{s!(\ell+s)!m!(m+\ell+2s+1)!} \left(\frac{Rk}{2}\right)^{2m+2\ell+4s} (\sin^2\alpha + \sin^2\alpha')^m$$
$$= \frac{1}{4\pi^2} \sum_{\ell=-\infty}^{\infty} \mathrm{e}^{i\ell\gamma} \sum_{s=\max(0,-\ell)}^{\infty} \frac{(\sin\alpha\sin\alpha')^{\ell+2s}}{s!(\ell+s)!} \left(\frac{Rk}{2}\right)^{2\ell+4s}$$
$$\times \sum_{m=0}^{\infty} \frac{(-1)^m (\sin^2\alpha + \sin^2\alpha')^m}{m!(m+\ell+2s+1)!} \left(\frac{Rk}{2}\right)^{2m}$$

If we rearrange the last sum over m we can note that this is the Taylor expansion of the Bessel functions. So we get

$$\sum_{m=0}^{\infty} \frac{(-1)^m \sqrt{\sin^2\alpha + \sin^2\alpha'}^{2m}}{m!(m+\ell+2s+1)!} \left(\frac{Rk}{2}\right)^{2m} = 2^{\ell+2s+1} \frac{J_{\ell+2s+1}(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})}{(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})^{\ell+2s+1}}$$

Equating coefficients, we can deduce that the Fourier coefficients of C_R are given by:

$$\widehat{C}_R(\alpha,\alpha',\ell) := \frac{1}{4\pi^2} \sum_{s=\max(0,-\ell)}^{\infty} \frac{(\sin\alpha\sin\alpha')^{\ell+2s}}{s!(\ell+s)!} \left(\frac{Rk}{\sqrt{2}}\right)^{2\ell+4s} \times \frac{J_{\ell+2s+1}(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})}{(Rk\sqrt{\sin^2\alpha+\sin^2\alpha'})^{\ell+2s+1}}. \tag{5.51}$$

Acknowledgments

Thanks to professor H.P. Urbach for suggesting this problem, as it unexpectedly involved different fields in deriving the solution.

References

[1] George E. Andrews, Richard Askey, and Ranjan Roy. *Special functions*. English. Cambridge: Cambridge University Press, 1999, xvi + 664 (see p. 106).

[2] R. de Bruin, H. P. Urbach, and S. F. Pereira. “On focused fields with maximum electric field components and images of electric dipoles”. In: *Opt. Express* 19.10 (May 2011), 9157–9171. DOI: 10.1364/OE.19.009157 (see p. 118).

[3] Gerald B. Folland. *Real analysis*. Second Edition. Pure and Applied Mathematics (New York). Modern techniques and their applications, A Wiley-Interscience Publication. John Wiley & Sons, Inc., New York, 1999, xvi+386 (see p. 115).

[4] Gerd Grubb. *Distributions and Operators*. Vol. 252. Graduate Texts in Mathematics. New York, NY: Springer New York, 2009. DOI: `10.1007/978-0-387-84895-2` (see p. 125).

[5] V. S. Ignatowsky. "Diffraction by a lens having arbitrary opening (in Russian)". In: *Trans. Opt. Inst. Petrograd* I (1919), paper IV (see p. 108).

[6] V. S. Ignatowsky. "Diffraction by a parabolic mirror having arbitrary opening (in Russian)". In: *Trans. Opt. Inst. Petrograd* I (1920), paper V (see p. 108).

[7] David G. Luenberger. *Optimization by vector space methods*. John Wiley & Sons, Inc., New York-London-Sydney, 1969, xvii+326 (see p. 89).

[8] Michael Reed and Barry Simon. *Methods of modern mathematical physics. I*. Second. Functional analysis. Academic Press, Inc. [Harcourt Brace Jovanovich, Publishers], New York, 1980, xv+400 (see pp. 92, 93, 101).

[9] B Richards and E Wolf. "Electromagnetic Diffraction in Optical Systems. II. Structure of the Image Field in an Aplanatic System". In: *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* 253.1274 (1959), 358–379. DOI: `10.1098/rspa.1959.0200` (see p. 108).

[10] Alastair Spence. "On the convergence of the Nyström method for the integral equation eigenvalue problem." English. In: *Numer. Math.* 25 (1975), 57–66. DOI: `10.1007/BF01419528` (see pp. 113, 114).

[11] H. P. Urbach and S. F. Pereira. "Focused fields of given power with maximum electric field components". In: *Phys. Rev. A* 79 (1 Jan. 2009), 013825. DOI: `10.1103/PhysRevA.79.013825` (see p. 86).

[12] E Wolf. “Electromagnetic Diffraction in Optical Systems. I. An Integral Representation of the Image Field”. In: *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences* 253.1274 (1959), 349–357. DOI: `10.1098/rspa.1959.0199` (see p. 108).

Summary

This dissertation consists out of rougly two parts, a mathematical parts and a physics part.

In the mathematical part we study the Ornstein–Uhlenbeck process with respect to the Gaussian measure. We focus on two areas. One is on "Gaussian" analogues of classical results in Harmonic analysis, and a second we study the integral kernels which arise from the function $z^k e^{tz}$ applied to the Ornstein–Uhlenbeck operator.

In Chapter 2 we look at the non-tangential maximal function for the Ornstein–Uhlenbeck semigroup and we prove analogues to classical results. An important distinction in this Chapter with the classical case is that the maximal function result for the Laplacian allows for all positive time t, whereas our result only holds for times $t \in (0, 1)$ depending on the position in space.

Chapter 3 is concerned with the integral kernel of $L^k e^{tL}$ for the Ornstein–

Uhlenbeck semigroup. We compute an explicit formula for this kernel related to the Mehler kernel. As an application we show several kernel bounds using our formula.

Finally, Chapter 4 concerns off-diagonal estimates related to the Ornstein–Uhlenbeck operator. It is well-known that these hold for the Laplacian with respect to the Lebesgue measure, but do these hold for the Ornstein–Uhlenbeck operator with respect to the Gaussian measure? It is known that we always would have L^2-L^2 bounds, even for all times, but in applications one often wants L^2-L^1 bounds. Even though these do hold for the Laplacian, we show that these cannot hold for the Ornstein–Uhlenbeck operator for small times $t \in (0,1)$. Moreover, our proof shows that letting the maximal t depend on the position in space will not work either.

In the second part of this dissertation we study a problem in theoretical optics.

Chapter 5 is concerned with the optimization of the electric field induced by light as a plane wave in a circle with given radius. We study the electric fields in the lens pupil and the focal region for several radii in the orde of magnitude of the wave length of the light used.

Samenvatting

Dit proefschrift bestaat uit twee delen, een wiskundig en een natuurkundig deel.

In het wiskundige deel bestuderen we het Ornstein–Uhlenbeck proces ten opzichte van de Gaussische maat. We concentreren ons op twee aspecten: ten eerste bestuderen we analoga van klassieke resultaten in de harmonische analyse, en ten tweede bestuderen we de werking van $z^k e^{tz}$ op de Ornstein–Uhlenbeck operator.

Hoofdstuk 2 beschouwt analoog aan het klassieke geval voor de Laplaciaan de niet-tangentiale maximaalfunctie maar dan voor de Ornstein–Uhlenbeck halfgroep. Een belangrijk onderscheid met het klassieke geval is hier dat de maximaalfunctie voor de Laplaciaan alle positive tijden t toestaat, waarbij ons resultaat dit enkel voor tijden $t \in (0,1)$ doet, waarbij deze ook nog afhangen van het punt in de ruimte.

In Hoofdstuk 3 bekijken we de integraalkernen van $L^k e^{tL}$ voor de Ornstein–

Uhlenbeck halfgroep. We berekenen een expliciete formule voor de kern welke gerelateerd is aan de Mehlerkern. Als toepassingen bekijken we verschillende kernongelijkheden met behulp van onze formule.

Als laatste wiskundig onderwerp beschouwen we in Hoofdstuk 4 de "off-diagonal estimates" gerelateerd aan de Ornstein–Uhlenbeck operator. Het is bekend dat deze gelden voor de Laplacian met de Lebesguemaat, maar gelden deze ook voor de Ornstein–Uhlenbeck operator met de Gaussische maat? Het is bekend dat we altijd L^2-L^2 off-diagonal estimates hebben, zelfs voor alle tijden $t > 0$, maar in toepassingen wil men vaak L^2-L^1 afschattingen. Zelfs al gelden deze voor de Laplaciaan tonen wij aan dat deze nooit zullen gelden voor de Ornstein–Uhlenbeck operator voor kleine $t \in (0, 1)$. Verder toont ons bewijs aan dat technieken zoals vaak gebruikt worden in het Gaussische geval zoals de tijd laten afhangen van het punt in de ruimte niet werken.

In het tweede deel van dit proefschrift bestuderen we een probleem in theoretische optica.

Hoofdstuk 5 beschouwt de optimalisatie van het elektrische veld geinduceerd door licht als een vlakke golf in een cirkel met gegeven straal. We bestuderen het electrische veld in de lens en in het focale gebied voor verschillende radii in de orde van grootte van golflengte van het invallende licht.

Acknowledgements

First of all I would like to thank my promotors Jan van Neerven and Paul Urbach for providing me with such interesting projects to work on. I truly wonder if I would have gotten this far without you, Jan, and I do not think there would have been a better promotor for me. Paul's challenging style further contributed greatly to the quality of my output.

Many thanks to all the PhD candidates from the 4^{th} floor who made the canteen lunches bearable, and my collaborators Mikko Kemppainen and Alex Amenta for their useful (in many way) distractions.

I intended to keep this very brief as I would never be able to compile an exhaustive list of people I owe my gratitude to. Nevertheless, I hope I will only write a PhD thesis once, so I would like to take the opportunity to single out a few people. My apologies if I forgot to mention any one of you, but I can do it much better verbally!

My board memberships at PNN, PromooD and VAWO taught me a whole lot more about life in general. There are many great people there, and I am thankful that I met anyone of them, but I would like to particulary mention

Charlotte, Victor, Filip, Ken and Marijtje.

Some friends I'd like to mention are my paranimphs Nathan and Remco. Thanks for putting up with all the things I will ask you to do. Thanks for the wonderful cover Fay and Lucas, I feel honoured that you wanted to create this for me. And last, but certainly not least a special thanks to Mirte for making me happy and inspiring me to stay present!

Curriculum Vitæ

Jonas Jan Bart Teuwen was born in Harelbeke, Belgium, on July 15th 1986. He completed his secondary education in 2004 at the Sint-Jozef Instituut in Schoten, Belgium. In 2006 he started his studies in Applied Mathematics at the Delft University of Technology to obtain his Master of Science degree in 2011 under supervision of Prof. dr. J.M.A.M. van Neerven. In the same year, he started his PhD research under the supervision of Prof. dr. J.M.A.M. van Neerven.

Part of this research was carried out at the Optics Research Group of the Delft University of Technology under the supervision of Prof. dr. H.P. Urbach.

List of Publications

1. **Jonas Teuwen**, *A note on the Gaussian maximal functions*, Indagationes Mathematicae **26.1**, pp. 106-112 (2015).
2. **Jonas Teuwen**, *On the integral kernels of derivatives of the Ornstein–Uhlenbeck semigroup (submitted)*, arXiv:`1509.05702`.
3. **Jonas Teuwen & Alex Amenta**, *A note on some local and non-local properties of the Ornstein–Uhlenbeck semigroup (in preparation)*.
4. **Jonas Teuwen & H.P. Urbach**, *Optimizing the electric energy density in a circle (in preparation)*.
5. **Jonas Teuwen & H.P. Urbach**, *A distributional approach to the Lorentz force applied to a surface of discontinuity of the dielectric permittivity (in preparation)*.