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# General Kernel Spectral Methods for Equilibrium Measures



## MASTER'S THESIS

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# Abstract

To be written.

This MMSC thesis will further explore general kernel spectral methods for finding equilibrium measures where initial progress made in [T. Gutleb, J. Carrillo and S. Olver 2022](#) and [T. S. Gutleb, José A. Carrillo and S. Olver 2022](#).

**Keywords:** Pairwise Interaction Potentials, Many-Body Systems, Particle Simulations, Swarming Behaviours, Equilibrium Measures, Spectral Methods, Orthogonal Polynomials

**Languages:** C++, Julia, Python

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# Chapter 1

## Introduction

This chapter will give a brief overview of the setting of the problem considered in this dissertation, motivate a few biological and physical examples, and set up some notational conventions.

### 1.1 Problem Setting

The present thesis is concerned with many-body systems, treating particles in an abstract sense as they could take the form of physical atoms, birds in a flock or fish in a school. Other examples include ant colonies and swarms of insects such as locusts. A swarm of animals, a set of coordinated entities, brings many advantages for its members. For example, they share water resistance or it is easier to find a mate within the swarm than otherwise. They also often mimic larger animals to fend off predators and swarming behaviour (“swarm intelligence”) plays an important role in this process. There are some disadvantages as well, like the accelerated spread of diseases or when resources are scarce, some swarm species even begin cannibalistic behaviour (D’Orsogna 2017).

From a more physical perspective, pair potentials  $K : \mathbb{R}^+ \mapsto \mathbb{R}$  provide a simple and computationally efficient way to approximate the interaction between two particles based solely on their distance (cf. Figure 1.1a as a simple illustration). The total potential of a system of  $N_p \geq 2$  particles  $U \in \mathbb{R}$  can be calculated by summing up the pair potentials  $U_{ij} \in \mathbb{R}$  between all pairs of particles

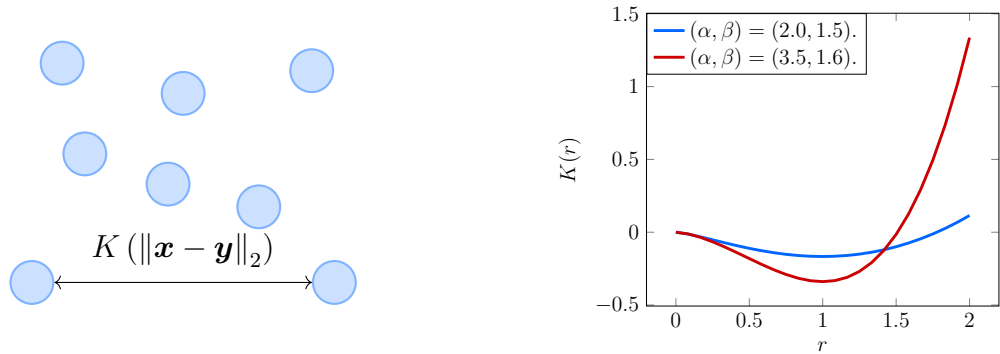
$$U = \sum_{i=1}^{N_p} \sum_{j=1, j \neq i}^{N_p} U_{ij} = \sum_{i=1}^{N_p} \sum_{j=1, j \neq i}^{N_p} K(\|\mathbf{x}_i - \mathbf{x}_j\|_2) ,$$

where  $\mathbf{x}_i \in \mathbb{R}^d$  represents the  $d$ -dimensional position of particle  $i$ , respectively.

Pairwise potentials can be used to approximate a wide range of interactions, including interatomic potentials in physics and computational chemistry. Common examples of pair potentials include the Lennard-Jones potential and the Morse potential, which are widely used in molecular dynamics simulations to study the behavior of atoms and molecules, as well as the Coulomb potential used to describe the interaction between two charges in electrodynamics. An example we will study is that of an attractive-repulsive interaction potential, where two power-law potentials compete with each other. For a given  $\alpha, \beta \in \mathbb{R} \setminus \{0\}$ , it is given by

$$K_{\alpha,\beta}(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}.$$

One can even consider the case where either  $\alpha$  or  $\beta$  is 0 in order to arrive at a log-term (José A. Carrillo and Huang 2017), using the convention that  $\frac{x^0}{0} := \log(x)$ <sup>1</sup>. If the repulsive term is stronger (so  $\beta > \alpha$ ), there is no equilibrium distribution as particles simply continue repelling each other out to infinity.



(a)  $N = 8$  particles interacting with one another (b) Plot of attractive-repulsive potential functions through the potential  $K(r)$ .

$$K_{\alpha,\beta}(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta} \text{ for different } \alpha, \beta.$$

From here on, we will refer to said swarm entities, be it fish, birds or atoms, as *particles*.

<sup>1</sup>Consider the Laurent series expansion of  $\frac{x^a}{a} = \frac{1}{a} + \log(x) + \frac{1}{2}a \log^2(x) + \mathcal{O}(a^2)$  in the limit as  $a \rightarrow 0^+$ . While this limit approaches  $\infty$  coming from the right and  $-\infty$  coming from the left due to the nature of the first term in the expansion, the only remaining term in it is  $\log(x)$  which is thereby chosen as a convention.

## 1.2 Notational Conventions

Let  $\mathbb{N}$  denote the natural numbers (positive integers) without 0 and let  $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$ . In the following, we will use **bold** notation for vectors, matrices will generally be denoted by a capital letter and scalars by a lowercase letter. We will frequently make use of the (Euclidean) 2-norm of a vector, as denoted by  $\|\cdot\|_2$ . So for a  $d$ -dimensional vector  $\mathbf{x} \in \mathbb{R}^d$  we have  $\|\mathbf{x}\|_2 := \sqrt{\sum_{k=1}^d x_k^2}$ .

One should also clarify the nature of a few of the integrals appearing in this thesis which are often performed over the closed unit ball  $B_1(\mathbf{x}) := \{\mathbf{y} \in \mathbb{R}^d \mid \|\mathbf{x} - \mathbf{y}\|_2 \leq 1\}$  centered at the origin  $\mathbf{x} = \mathbf{0}$ . These volume integrals (often ended by  $d^d y$  or  $dV$ ) over the  $d$ -dimensional unit ball shall be written as

$$\int_{B_1(\mathbf{0})} d\mathbf{y},$$

where  $\mathbf{y} \in \mathbb{R}^d$  is the integration variable. Note that some definitions of  $B_1(\mathbf{x})$  are open sets, leaving out the shell  $\{\mathbf{y} \in \mathbb{R}^d \mid \|\mathbf{x} - \mathbf{y}\|_2 = 1\}$ . The choice of definition does not matter for our purposes as the shell, a hyperplane of Lebesgue measure 0, does not contribute to the integral.

All numerical plots and figures in this thesis were generated using the Makie visualisation tool ([Danisch and Krumbiegel 2021](#)), an open-source package available for the Julia computing language ([Bezanson et al. 2017](#)).

# Just Notes

This chapter's purpose is the collection of notes, and it will not be included in the final dissertation.

## Special Functions we like

**Pochhammer's falling symbol**  $(x)_n := \prod_{k=0}^{n-1} (x - k)$ .

**Pochhammer's rising symbol**  $(x)^n := \prod_{k=0}^{n-1} (x + k)$ .

**Generalised hypergeometric series**

$${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z) := \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{z^n}{n!}.$$

**(Gaussian) Hypergeometric function**

$${}_2F_1(a, -n; c; z) = \sum_{j=0}^n (-1)^j \binom{n}{j} \frac{(a)_j}{(c)_j} z^j.$$

(A special case of the hypergeometric series with  $p = 2$ ,  $q = 1$ ).

**Jacobi (=hypergeometric) polynomials**

$$P_n^{(\alpha, \beta)}(z) := \frac{(\alpha + 1)_n}{n!} {}_2F_1\left(-n, 1 + \alpha + \beta + n; \alpha + 1; \frac{1}{2}(1 - z)\right).$$

**Gegenbauer (=ultraspherical) polynomials**

$$C_n^{(\lambda)}(z) := \frac{(2\lambda)_n}{n!} {}_2F_1\left(-n, 2\lambda + n; \lambda + \frac{1}{2}; \frac{1 - z}{2}\right) = \frac{(2\lambda)_n}{(\lambda + \frac{1}{2})_n} P_n^{(\lambda-1/2, \lambda-1/2)}(x).$$



They satisfy a three-term recurrence relation (as all orthogonal polynomials do!)

$$\begin{aligned} C_0^{(\lambda)}(x) &= 1 \\ C_1^{(\lambda)}(x) &= 2\lambda x \\ (n+1)C_{n+1}^{(\lambda)}(x) &= 2(n+\lambda)x C_n^{(\lambda)}(x) - (n+2\lambda-1)C_{n-1}^{(\lambda)}(x). \end{aligned}$$

From Wikipedia: In spectral methods for solving differential equations, if a function is expanded in the basis of Chebyshev polynomials and its derivative is represented in a Gegenbauer/ultraspherical basis, then the derivative operator becomes a diagonal matrix, leading to fast banded matrix methods for large problems (S. Olver and Townsend 2013).

**Three-term recurrence relationship** F. Olver et al. 2018, p. 18.9.1:

$$x C_n^{(\lambda)}(x) = \frac{(n+2\lambda-1)}{2(n+\lambda)} C_{n-1}^{(\lambda)}(x) + \frac{n+1}{2(n+\lambda)} C_{n+1}^{(\lambda)}(x). \quad (1.1)$$

### 1.2.1 Theorem: Two term recurrence of $Q^\alpha$

The integral operator

$$Q^\alpha[u](x) = \int_{-1}^1 |x-y|^\alpha u(y) dy$$

satisfies a two-term recurrence relationship when acting on the ultraspherical polynomials  $C_n^{(\lambda)}(y)$  with weight  $w(y) = (1-y^2)^{\lambda-\frac{1}{2}}$  such that

$$x Q^\alpha[w C_n^{(\lambda)}](x) = \kappa_1 Q^\alpha[w C_{n-1}^{(\lambda)}](x) + \kappa_2 Q^\alpha[w C_{n+1}^{(\lambda)}](x),$$

where  $n \geq 2$  and with the constants

$$\begin{aligned} \kappa_1 &= \frac{(n-\alpha-1)(2\lambda+n-1)}{2n(\lambda+n)}, \\ \kappa_2 &= \frac{(n+1)(2\lambda+n+\alpha+1)}{2(\lambda+n)(2\lambda+n)}. \end{aligned}$$

# Chapter 2

## Particle Interaction Theory

As mentioned in the introduction.

Lennard-Jones is an **intermolecular** potential. So length-scale is between-molecules. Therefore, the only relevant interaction is the electromagnetic one. The strong force keeps protons in the nucleus together (a force much stronger than the electromagnetic one).

**Definition:  $N_p$ -Body System** (a set of particles with position and velocity) Each particle  $i = 1, \dots, N_p$  at position  $\mathbf{x}_i \in \mathbb{R}^d$  and time  $t \in \mathbb{R}^+$  follows

$$\frac{d^2 \mathbf{x}_i}{dt^2} = f \left( \left\| \frac{d\mathbf{x}_i}{dt} \right\|_2 \right) \frac{d\mathbf{x}_i}{dt} - \frac{1}{N} \sum_{j=1, i \neq j}^N \nabla K \left( \|\mathbf{x}_i - \mathbf{x}_j\|_2 \right),$$

for reference see, for example, (T. Gutleb, J. Carrillo and S. Olver 2022; T. S. Gutleb, José A. Carrillo and S. Olver 2022). For now, we only consider the case without an external potential  $V(\mathbf{x})$ .

**Inertia / kinetic energy** Each particle has inertia and its kinetic energy (“second moment”<sup>1</sup>) is given by

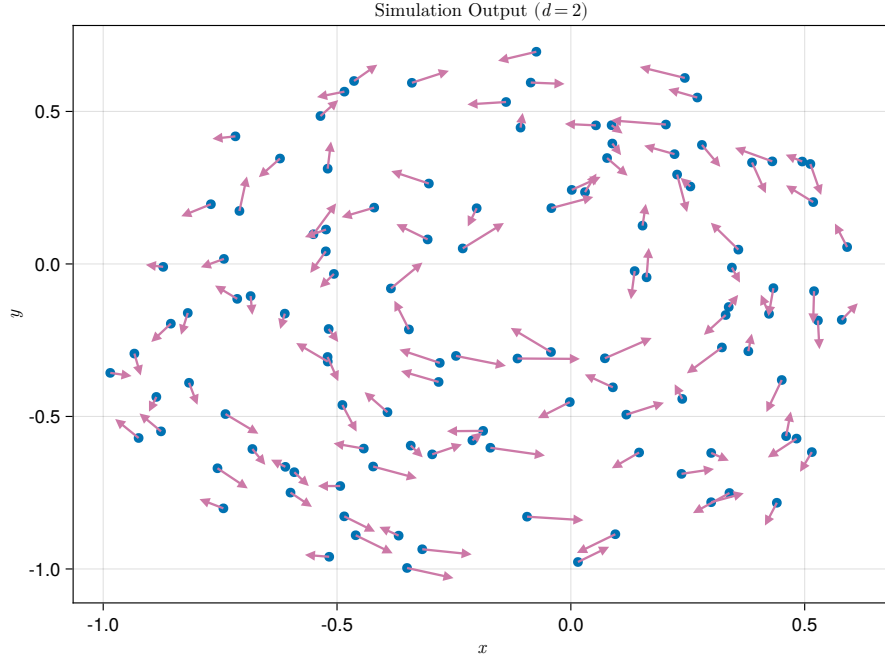
$$E_{\text{kin},i} = \frac{\mathbf{p}_i^2}{2m} = \frac{(m\mathbf{v}_i)^2}{2m} = \frac{1}{2}m \|\mathbf{v}_i\|_2^2.$$

In the absence of an external potential, the total energy is given by  $E = E_{\text{kin}} + U$ .

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<sup>1</sup>In kinetic theory, the 0th moment is the mass  $m$  of a particle, the first moment is the momentum  $\mathbf{p}$  and the second moment is its kinetic energy.

Potentials motivating a force  $F = -\nabla U$



**Figure 2.1:** Position and velocity of particles in the simulation.

## 2.1 Continuous Limit

The total energy, in the continuous limit as  $N_p \rightarrow \infty$ , becomes

$$E = \frac{1}{2} \iint K(\|\mathbf{x} - \mathbf{y}\|_2) \, d\rho(\mathbf{x}) \, d\rho(\mathbf{y}),$$

where  $d\rho = \rho(\mathbf{x})d\mathbf{x}$  is a measure (the equilibrium distribution) chosen such that

$$M = \int d\rho = \int_{\text{supp}(\rho)} \rho(\mathbf{x}) \, d\mathbf{x} = 1.$$

## 2.2 Self-Propulsion

Makes it active matter.

Self-propulsion and friction could be modelled as a quadratic of the form

$$f(v_i) = 1.6 - 0.5v_i^2,$$

where  $v_i := \|\mathbf{v}_i\|_2 = \left\| \frac{d\mathbf{x}_i}{dt} \right\|_2$ . Show reproduced plots from [D’Orsogna et al. 2006](#).

**To be included.**

## 2.3 Kinetic Theory: The Vlasov Equation

A very common tool in Plasma physics.

$$\frac{\partial f}{\partial t} + \frac{d\mathbf{r}}{dt} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{d\mathbf{p}}{dt} \cdot \frac{\partial f}{\partial \mathbf{p}} = 0,$$

This is the collisionless Boltzmann equation. Vlasov replaces the collision term with long-range interactions.

### 2.3.1 Theorem: Liouville's

Says that phase-space volume is conserved in situations of a pure particle-particle interaction.

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^n \left( \frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = 0.$$

## 2.4 Vicsek Model

For the study of active matter (a number of individual agents).

## 2.5 Swarming

A 2010 paper by [Cavagna et al.](#) showed the surprising result that correlation between movement of individual starlings in bird flocks over Rome is scale-free. In contrast to the assumption that birds only mirror their neighbours' behaviour and swarming behaviour emerges as a result of that, this observation suggests that bird flocks exert collective behaviour beyond local interactions.

The change in the behavioral state of one animal affects and is affected by that of all other animals in the group, no matter how large the group is ([Cavagna et al. 2010](#)).

This work was done by individually tracking each starling in the flock and using tracking algorithms to represent their 3 dimensional positions and velocities.

# Chapter 3

## Particle Simulator

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is there to solve problems in [[Particle Interaction Theory]].

### 3.0.1 Structure

- Talk about different integration methods
- Leap-Frog Integration
- Screenshot of GUI

### 3.0.2 Available Methods:

- [[Integration Routine]]
  - Simple Forward Integration
  - Improvements: Multistep methods
  - [[Leapfrog Integration]]
- [[Fast Multipole Method]]
- [[Multigrid Methods]]

### 3.0.3 Available Solvers:

- LAMMPS ancient
- [Gromacs](#) has nice homepage

- [OpenMM](#) also has nice homepage
- [OpenFPM](#)
- [\[\[General Kernel Spectral Method\]\]](#) for [\[\[Equilibrium Measures\]\]](#)

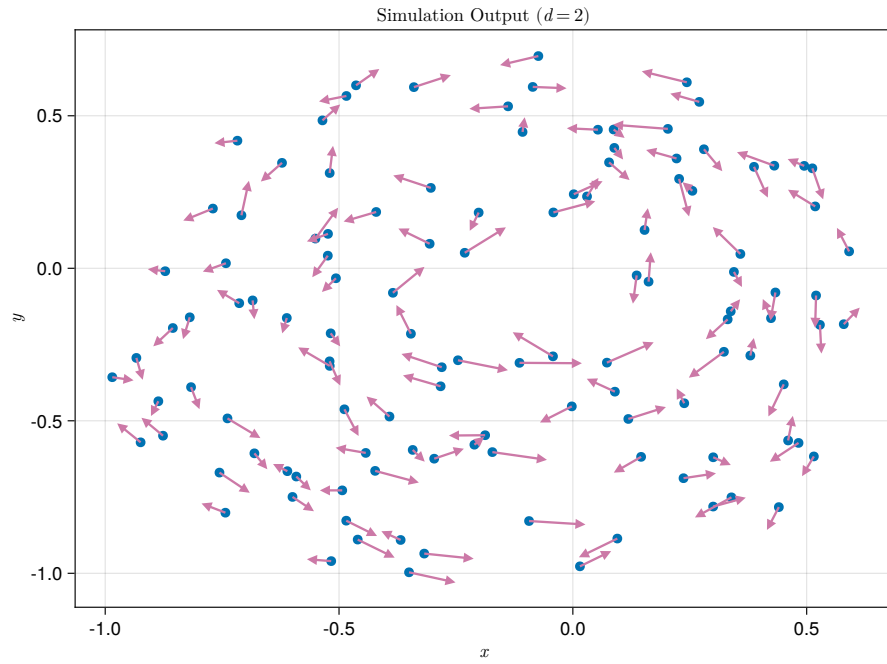
### 3.0.4 Implementations in [\[\[My Dissertation\]\]](#):

- [\[\[C++ Particle Integrator with GUI\]\]](#)

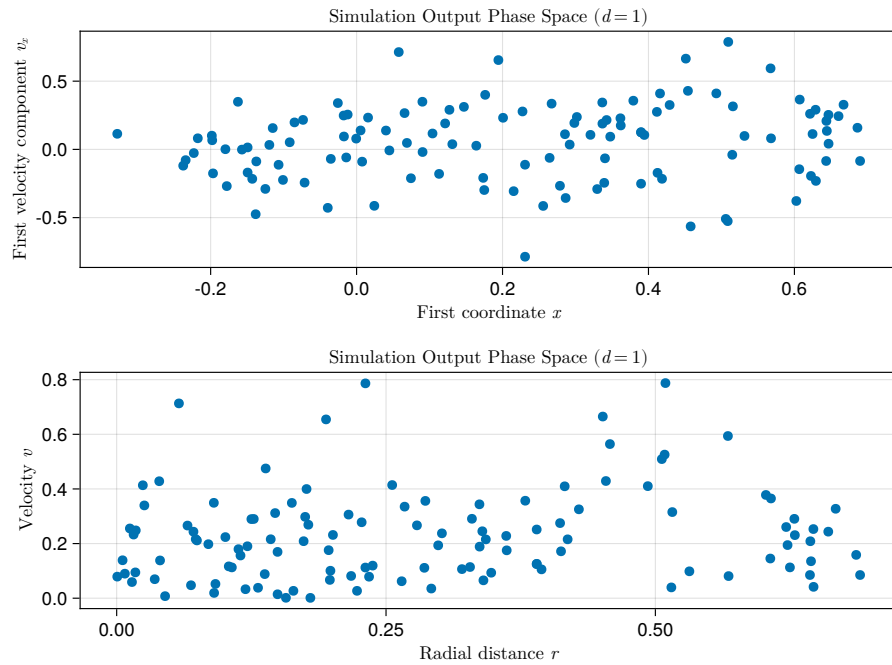
Nice introduction [here](#). Maybe compare with [Advanced HMC](#)?



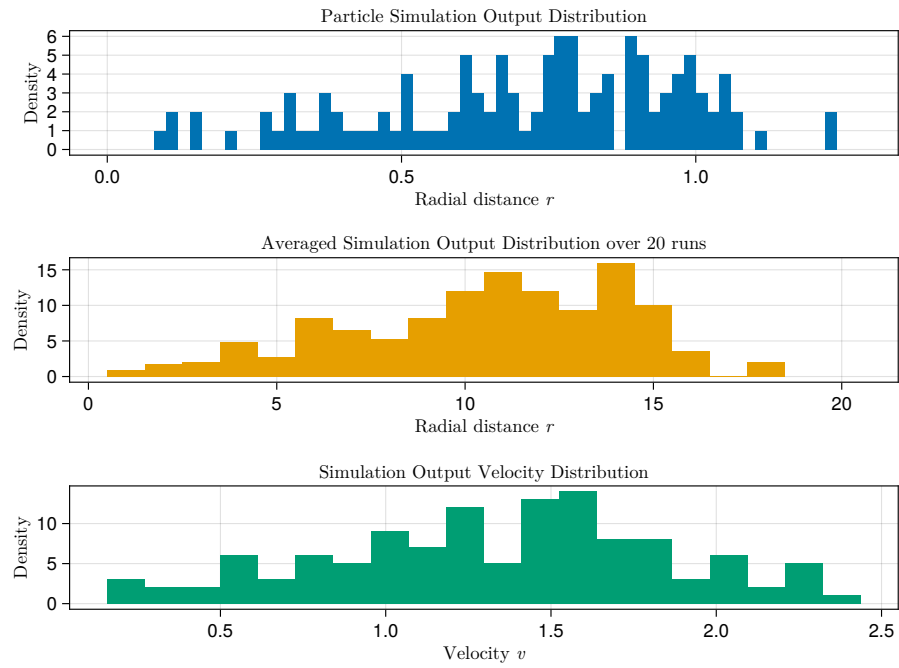
**Figure 3.1:** Screenshot of the GUI



**Figure 3.2:** Position and velocity of particles in the simulation.



**Figure 3.3:** Position and velocity of particles in the simulation visualised as a phase space plot.

**Figure 3.4:** Position Histogram



# Chapter 4

## Spectral Method

### 4.1 Content

solves an [[Integral Equation]] or [[Differential Equation]] by assuming a solution of the form

$$\rho(x) = \sum_{k=1}^N \rho_k b_k(x)$$

where  $\{b_k\}$  is a basis of functions.

#### 4.1.1 Structure

- Introduce [[Chebyshev Polynomials]], [[Gegenbauer Polynomials|Ultraspherical Polynomials]], [[Jacobi Polynomials]], etc.
- Describe the method
- Talk about the resulting [[Operator]].
  - [[Derivation of In-Operator Recurrence]]
- Numerical Analysis ([[Bound on the Error]])
- Show results here? Or in extra results chapter?

## 4.2 Definitions

### 4.2.1 Definition: Ansatz

$$\rho(\mathbf{x}) = \left(1 - \|\mathbf{x}\|_2^2\right)^{m - \frac{\alpha+d}{2}} \sum_{k=1}^N P_k^{(a,b)}(2\|\mathbf{x}\|_2^2 - 1)$$

### 4.2.2 Definition: Bound on the Error

- [ ] How does one look at this topic? We should have [[Spectral Convergence]], hopefully.

### 4.2.3 Definition: Chebyshev Polynomials

Of the first kind:

$$T_k(x)$$

Of the second kind:

$$U_k(x)$$

Also have a [[Three-Term Recurrence Relationship]].

Based on the Three-Term Recurrence Relationship (cf. Definition 4.2.16).

One can even determine an explicit relationship between the coefficients in the Jacobi expansion by considering the Jacobi Matrix (cf. Definition 4.2.10).

Considering the operator  $\hat{Q}^\beta[\rho]$  as in Theorem 4.2.1, from the ansatz  $\rho(\mathbf{x})$  (cf. Definition 4.2.1) we have

$$\hat{Q}^\beta(x) = \sum_{k=0}^{N-1} \rho_k \int_{B_1(\mathbf{0})} \|\mathbf{x} - \mathbf{y}\|_2^\beta (1 - \|\mathbf{y}\|_2^2)^a P_k^{(a,b)} (2 \|\mathbf{y}\|_2^2 - 1) d\mathbf{y}. \quad (4.1)$$

We are now interested in a numerical representation of the operator  $\hat{Q}^\beta$  acting on the function  $\rho \in L^2$ , so an equivalent (linear) operator  $Q^\beta : \mathbb{R}^N \mapsto \mathbb{R}^N$  acting on the coefficients  $\rho_k \in \mathbb{R}$ ,  $k = 1, \dots, N$ . As every finite-dimensional linear operator must have a matrix representation, we are looking for a  $Q^\beta \in \mathbb{R}^{N \times N}$  such that

$$\hat{Q}^\beta[\rho](\mathbf{x}) = \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \cdot Q^\beta \boldsymbol{\rho},$$

where  $\mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \in \mathbb{R}^N$  is the vector of Jacobi polynomials  $P_0^{(a,b)}(x)$ ,  $P_1^{(a,b)}(x)$ , ...,  $P_{N-1}^{(a,b)}(x)$  evaluated at  $2 \|\mathbf{x}\|_2^2 - 1$  as introduced in and after Definition 4.2.11.

Therefore, starting from Equation (4.2), we obtain

$$\begin{aligned} \hat{Q}^\beta[\rho](\mathbf{x}) &= \sum_{k=0}^{N-1} \rho_k \hat{Q}^\beta[wP_k](\mathbf{x}) = \sum_{k=0}^{N-1} \rho_k \sum_{j=0}^{N-1} q_{kj} P_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \\ &= \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \rho_k q_{kj} P_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1), \end{aligned}$$

which we will rewrite in matrix-form,

$$\begin{aligned} \hat{Q}^\beta[\rho](\mathbf{x}) &= \mathbf{P}(\mathbf{x}) \cdot \begin{pmatrix} \sum_{k=0}^{N-1} \rho_k q_{k,1} \\ \vdots \\ \sum_{k=0}^{N-1} \rho_k q_{k,N} \end{pmatrix} = \mathbf{P}(\mathbf{x}) \cdot \underbrace{\begin{pmatrix} q_{11} & \dots & q_{1N} \\ \vdots & \ddots & \vdots \\ q_{N1} & \dots & q_{NN} \end{pmatrix}}_{=: Q^\beta} \begin{pmatrix} \rho_0 \\ \vdots \\ \rho_{N-1} \end{pmatrix} \\ &= \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \cdot Q^\beta \boldsymbol{\rho} \end{aligned}$$

where we used  $\mathbf{P}(\mathbf{x}) = \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1)$  as a shorthand giving us the form of the operator matrix. Each value  $q_{kj}$  in it is therefore chosen to satisfy

**4.2.4 Definition: Equilibrium Measures**

Are a Measure (cf. ??)

$$\rho : \mathbb{R} \mapsto \mathbb{R}, \rho(x)$$

- [ ] Need to fix this definition Can be computed using [EquilibriumMeasures.jl](#)

**4.2.5 Definition: Function Space**

To be defined, but the space our coefficients are in. Could be

$$L^2 := \{f : \mathbb{R} \mapsto \mathbb{R} | f \text{ square integrable?}\}$$

**4.2.6 Definition: Gaussian Hypergeometric Function**

Written as

$${}_2F_1(a, b; c; z)$$

**4.2.7 Definition: Gegenbauer Polynomials**

alias: Ultraspherical Polynomials

Are a special case of the Jacobi Polynomials (cf. Definition 4.2.11) and form an Orthonormal Basis (cf. ??) under the weight given by

$$w(x) = (1 + x)^\alpha$$

**4.2.8 Definition: Generalised Hypergeometric Series**

Is given by

$${}_pF_q$$

Special Case: [[Gaussian Hypergeometric Function]]. The definition involves the Rising Factorial (cf. Definition 4.2.14) (Pochhammer Symbol).

**4.2.9 Definition: Integration Routine**

Could be done using [Cubature](#). Otherwise, just Forward Euler.

**4.2.10 Definition: Jacobi Matrix**

aliases: Jacobi Operator

The **Jacobi operator** is the matrix  $X \in \mathbb{R}^{N \times N}$  satisfying

$$x \cdot P(x) = P(x) \cdot X^T$$

**4.2.11 Definition: Jacobi Polynomials**

Let  $P^{(a,b)} : \mathbb{C} \mapsto \mathbb{C}$  with

$$P_n^{(a,b)}(x) = \frac{(a+1)_n}{n!} {}_2F_1\left(-n, 1+a+b+n; a+1; \frac{1}{2}(1-x)\right)$$

So are defined using the Gaussian Hypergeometric Function (cf. Definition 4.2.6) and the Pochhammer symbol. Which is equivalent to

$$P_n^{(a,b)}(x) = \frac{\Gamma(a+n+1)}{n! \Gamma(a+b+n+1)} \sum_{m=0}^n \binom{n}{m} \frac{\Gamma(a+b+n+m+1)}{\Gamma(a+m+1)} \left(\frac{x-1}{2}\right)^m.$$

where  $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$  (with  $\Re(x) > 0$ ) is the gamma function <sup>1</sup>.

Gegenbauer Polynomials (cf. Definition 4.2.7) are a special case. And Chebyshev Polynomials (cf. Definition 4.2.3) are a special case of them.

Following from this definition,

$$\begin{aligned} P_0^{(a,b)}(x) &= 1 \\ P_1^{(a,b)}(x) &= (a+1) + (a+b+2) \frac{x-1}{2} \end{aligned}$$

and so on. Note that obviously,  $\deg(P_k^{(a,b)}) = k$ .

**4.2.1 Nice Spectral Properties**

- Differentiation
- Three-Term Recurrence
- why are they better than just Chebyshev?

Note that in this manuscript we will use the dot-product notation

$$f(x) = \sum_{k=0}^{N-1} f_k P_k^{(a,b)}(x) \quad \Leftrightarrow \quad f(x) = \mathbf{f} \cdot \mathbf{P}^{(a,b)}(x),$$

<sup>1</sup>Recall that for integer arguments  $k \in \mathbb{N}$ , it equals the factorial of  $(k-1)$  so  $\Gamma(k) = (k-1)!$ .

to express that a function  $f$  is a linear combination of basis polynomials with coefficients  $\mathbf{f} = (f_0, \dots, f_{N-1})^T \in \mathbb{R}^N$ . So  $\mathbf{P}^{(a,b)}(x) \in \mathbb{R}^N$  is the vector of Jacobi polynomials  $P_0^{(a,b)}(x), P_1^{(a,b)}(x), \dots, P_{N-1}^{(a,b)}(x)$ .

Jacobi polynomials  $P_n^{(a,b)}(x)$  are orthogonal on  $[-1, 1]$  w.r.t. the weight function

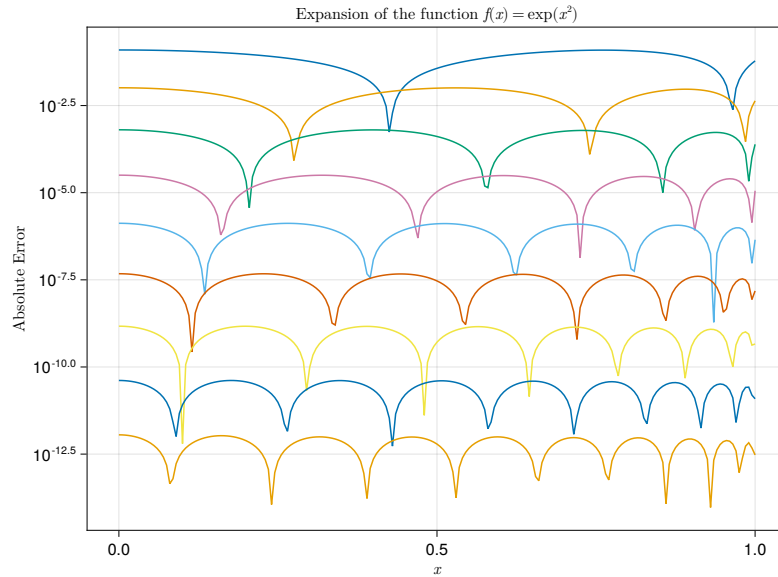
$$w^{(a,b)}(x) = (1-x)^a(1+x)^b,$$

so they satisfy

$$\int_{-1}^1 (1-x)^a(1+x)^b P_n^{(a,b)} P_m^{(a,b)} dx = \frac{2^{a+b+1} \Gamma(a+n+1) \Gamma(b+n+1)}{n! (a+b+2n+1) \Gamma(a+b+n+1)} \delta_{n,m},$$

with  $a, b > -1$ , which uniquely determines  $P_n^{(a,b)}(x)$ . The special case of  $a = b$  corresponds to the ultraspherical or Gegenbauer polynomials, while the case  $a = b = 0$  corresponds to the Legendre polynomials [F. Olver et al. 2018](#).

- This basis yields a **sparse**, and in particular, **banded** operator.



**Figure 4.1:** Convergence of Jacobi polynomial expansion. Convergence speed according to theory is: TODO.

#### 4.2.12 Definition: Operator

Either the attractive or the repulsive operator can be sparse.

Obtained using [\[\[Theorem 2.16\]\]](#). Derivation of the exact row/column form on paper ( `#include` in My Dissertation (cf. `??`))

- `[ ]` What does the solver look like for other kernels?

**4.2.13 Definition: Orthogonal Polynomials**

Are univariate polynomials

$$p : \mathbb{R} \mapsto \mathbb{R}, \quad p(x) = \sum_{k=1}^N c_k x^k.$$

that form an Orthonormal Basis (cf. ??) under some inner product.

**4.2.14 Definition: Rising Factorial**

alias: Pochhammer Symbol

Given by

$$(x)_n = \prod_{k=0}^{n-1} (x + k).$$

**4.2.15 Definition: Spectral Convergence**

**Definition 3.6** (Convergence at spectral speed) An  $N$ -point approximation  $\varphi_N$  of a function  $f$  converges to  $f$  at spectral speed if  $|\varphi_N - f|$  decays pointwise in  $[-1, 1]$  faster than  $O(N^{-p})$  for any  $p = 1, 2, \dots$  so  $p \in \mathbb{N}$ .

Source: [https://www.damtp.cam.ac.uk/user/cbs31/Teaching\\_files/c11.pdf](https://www.damtp.cam.ac.uk/user/cbs31/Teaching_files/c11.pdf).

**4.2.16 Definition: Three-Term Recurrence Relationship**

All Orthogonal Polynomials (cf. Definition 4.2.13) have (at least) a three-term recurrence relationship.

- [ ] how could I prove that?

### 4.2.1 Theorem: Integration Theorem that needs a name

On the  $d$ -dimensional unit ball  $B_1$  the power law potential, with power  $\alpha \in (-d, 2 + 2m - d)$ ,  $m \in \mathbb{N}_0$  and  $\beta > -d$ , of the  $n$ -th weighted radial Jacobi polynomial

$$(1 - |y|^2)^{m - \frac{\alpha+d}{2}} P_n^{(m - \frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2 - 1)$$

reduces to a Gaussian hypergeometric function as follows:

$$\begin{aligned} & \int_{B_1} |x - y|^\beta (1 - |y|^2)^{m - \frac{\alpha+d}{2}} P_n^{(m - \frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2 - 1) dy \\ &= \frac{\pi^{d/2} \Gamma(1 + \frac{\beta}{2}) \Gamma(\frac{\beta+d}{2}) \Gamma(m+n - \frac{\alpha+d}{2} + 1)}{\Gamma(\frac{d}{2}) \Gamma(n+1) \Gamma(\frac{\beta}{2} - n + 1) \Gamma(\frac{\beta-\alpha}{2} + m+n+1)} {}_2F_1 \left( n - \frac{\beta}{2}, \quad -m - n + \frac{\alpha-\beta}{2}; \frac{d}{2}; |x|^2 \right). \end{aligned}$$

Theorem 4.2.1 gives an explicit expression for the main integral  $Q^\beta : L \mapsto L$ , an operator from the Function Space  $L$  to the function space  $L$ , we are interested in:

$$\hat{Q}^\beta[\rho](x) = \int_{B_1} |x - y|^\beta (1 - |y|^2)^{m - \frac{\alpha+d}{2}} P_n^{(m - \frac{\alpha+d}{2}, \frac{d-2}{2})}(2|y|^2 - 1) dy$$

which is used to construct the Spectral Method Operator  $Q^\beta$  (cf. Definition 4.2.12), acting on the coefficients  $\rho$ .

## 4.3 Derivation of Operator

Based on the Three-Term Recurrence Relationship (cf. Definition 4.2.16).

One can even determine an explicit relationship between the coefficients in the Jacobi expansion by considering the Jacobi Matrix (cf. Definition 4.2.10).



Considering the operator  $\hat{Q}^\beta[\rho]$  as in Theorem 4.2.1, from the ansatz  $\rho(\mathbf{x})$  (cf. Definition 4.2.1) we have

$$\hat{Q}^\beta(x) = \sum_{k=0}^{N-1} \rho_k \int_{B_1(\mathbf{0})} \|\mathbf{x} - \mathbf{y}\|_2^\beta (1 - \|\mathbf{y}\|_2^2)^a P_k^{(a,b)} (2 \|\mathbf{y}\|_2^2 - 1) d\mathbf{y}. \quad (4.2)$$

We are now interested in a numerical representation of the operator  $\hat{Q}^\beta$  acting on the function  $\rho \in L^2$ , so an equivalent (linear) operator  $Q^\beta : \mathbb{R}^N \mapsto \mathbb{R}^N$  acting on the coefficients  $\rho_k \in \mathbb{R}$ ,  $k = 1, \dots, N$ . As every finite-dimensional linear operator must have a matrix representation, we are looking for a  $Q^\beta \in \mathbb{R}^{N \times N}$  such that

$$\hat{Q}^\beta[\rho](\mathbf{x}) = \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \cdot Q^\beta \boldsymbol{\rho},$$

where  $\mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \in \mathbb{R}^N$  is the vector of Jacobi polynomials  $P_0^{(a,b)}(x)$ ,  $P_1^{(a,b)}(x)$ , ...,  $P_{N-1}^{(a,b)}(x)$  evaluated at  $2 \|\mathbf{x}\|_2^2 - 1$  as introduced in and after Definition 4.2.11.

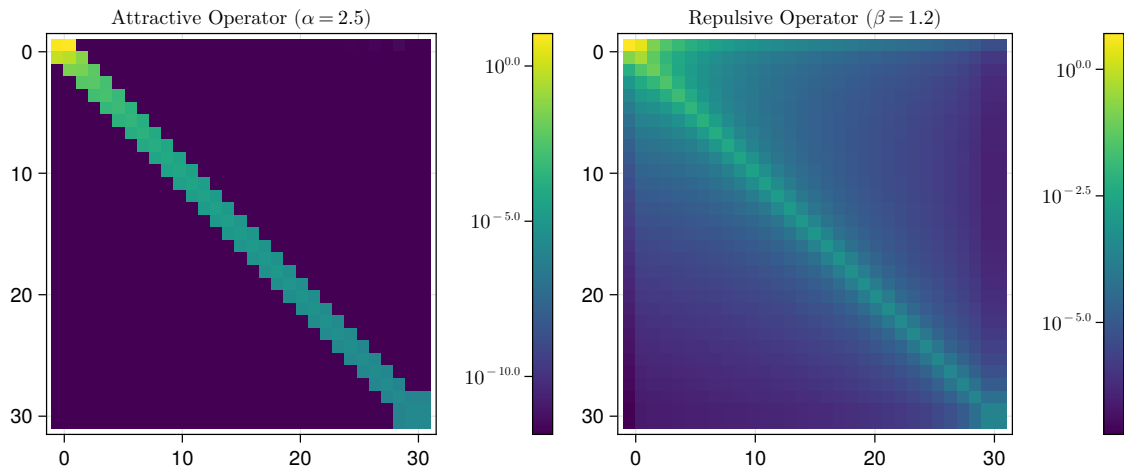
Therefore, starting from Equation (4.2), we obtain

$$\begin{aligned} \hat{Q}^\beta[\rho](\mathbf{x}) &= \sum_{k=0}^{N-1} \rho_k \hat{Q}^\beta[wP_k](\mathbf{x}) = \sum_{k=0}^{N-1} \rho_k \sum_{j=0}^{N-1} q_{kj} P_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \\ &= \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} \rho_k q_{kj} P_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1), \end{aligned}$$

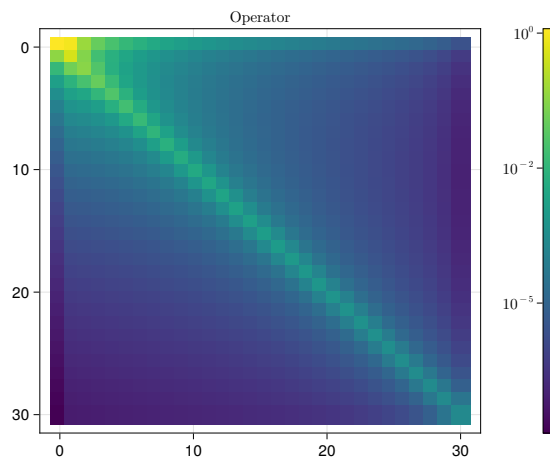
which we will rewrite in matrix-form,

$$\begin{aligned} \hat{Q}^\beta[\rho](\mathbf{x}) &= \mathbf{P}(\mathbf{x}) \cdot \begin{pmatrix} \sum_{k=0}^{N-1} \rho_k q_{k,1} \\ \vdots \\ \sum_{k=0}^{N-1} \rho_k q_{k,N} \end{pmatrix} = \mathbf{P}(\mathbf{x}) \cdot \underbrace{\begin{pmatrix} q_{11} & \dots & q_{1N} \\ \vdots & \ddots & \vdots \\ q_{N1} & \dots & q_{NN} \end{pmatrix}}_{=: Q^\beta} \begin{pmatrix} \rho_0 \\ \vdots \\ \rho_{N-1} \end{pmatrix} \\ &= \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1) \cdot Q^\beta \boldsymbol{\rho} \end{aligned}$$

where we used  $\mathbf{P}(\mathbf{x}) = \mathbf{P}_k^{(a,b)} (2 \|\mathbf{x}\|_2^2 - 1)$  as a shorthand giving us the form of the operator matrix. Each value  $q_{kj}$  in it is therefore chosen to satisfy

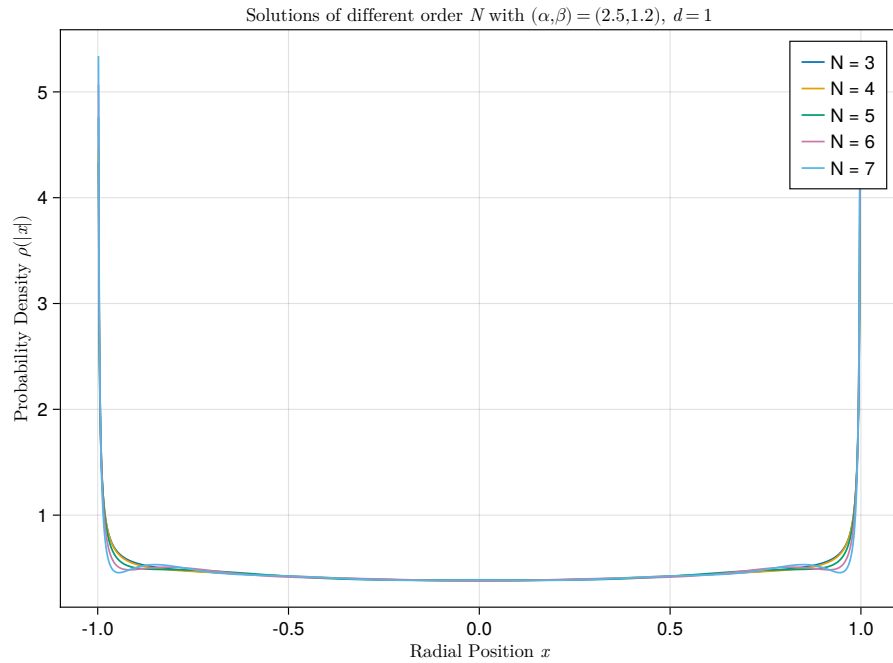


**Figure 4.2:** The attractive and repulsive operators (matrices), values are in log10-scale.



**Figure 4.3:** Operator

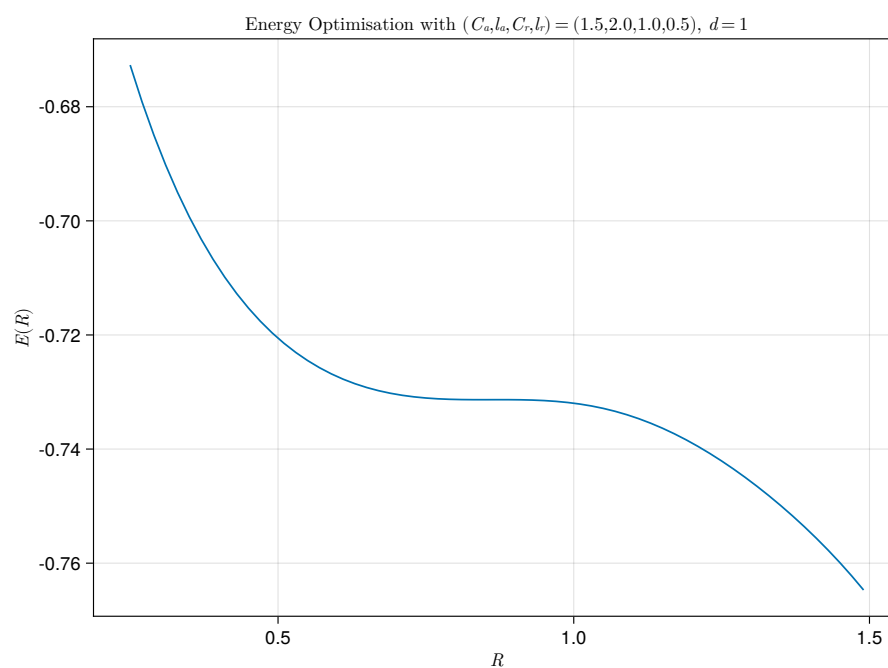
## 4.4 Results



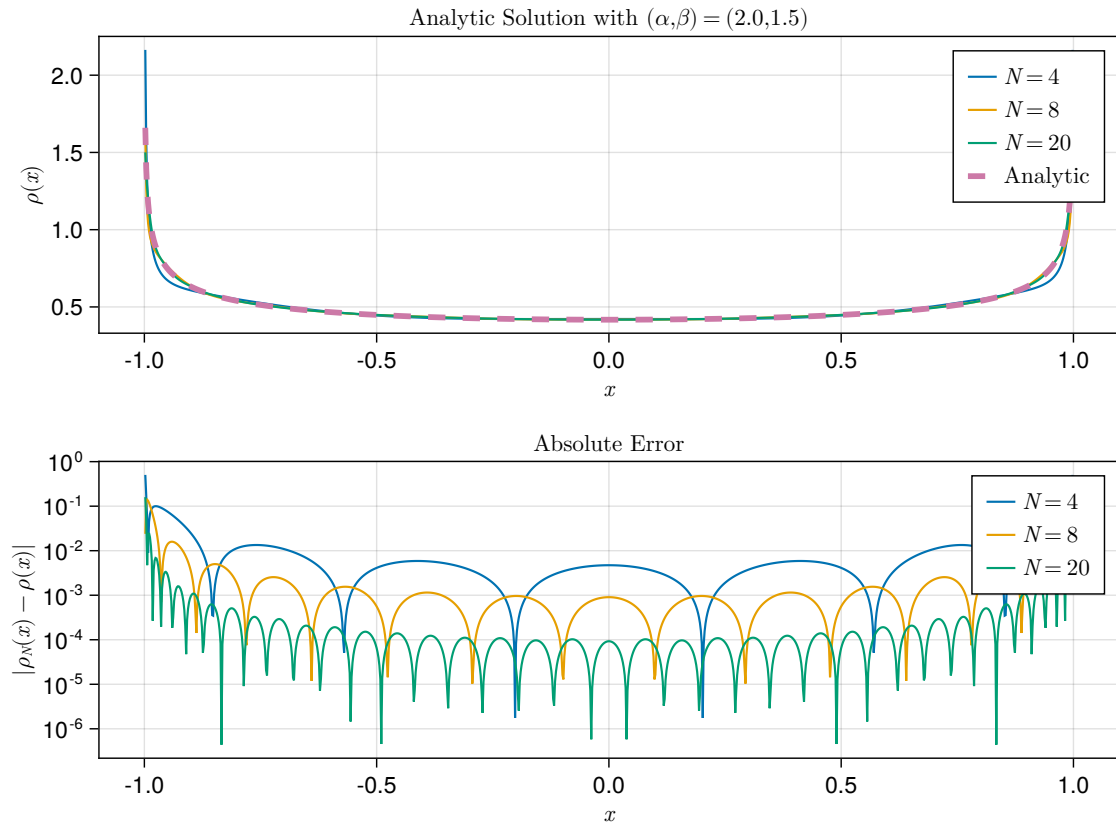
**Figure 4.4:** Solutions of increasing orders

## 4.5 Outer Optimisation Routine

Perhaps use [[Clarabel]] if we have a convex optimisation problem?

**Figure 4.5:** Outer Optimisation

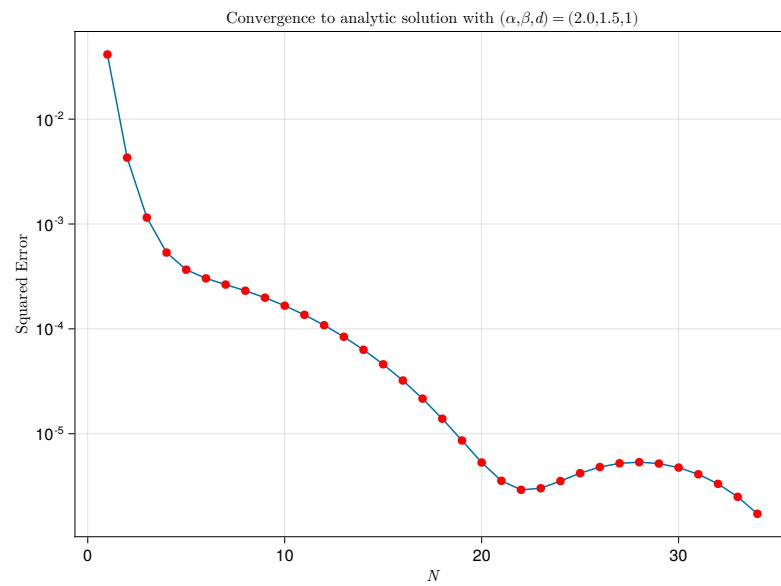
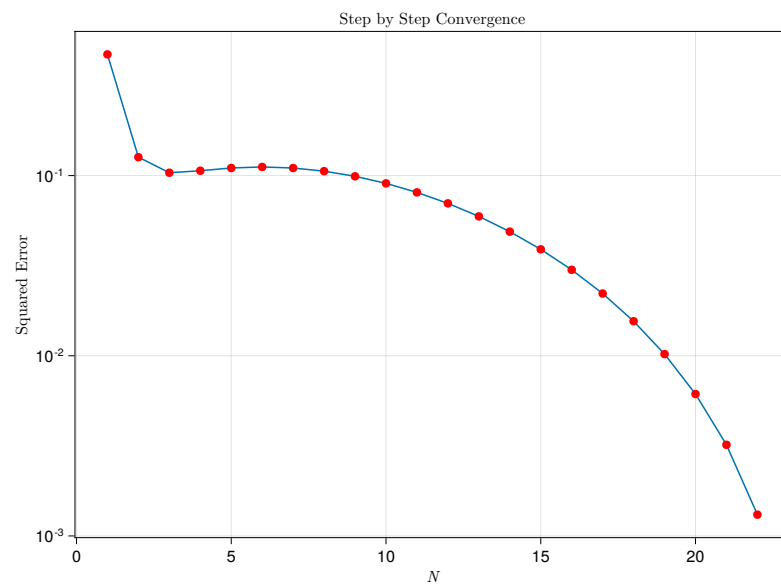
## 4.6 Analytic Solutions

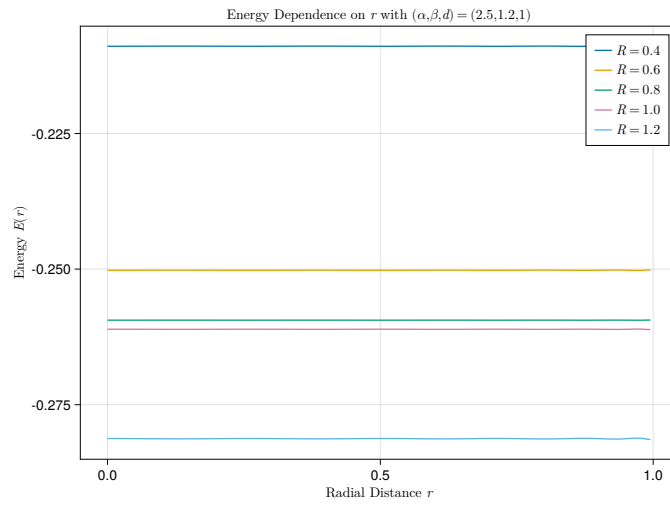


**Figure 4.6:** Analytic solution and comparison to numerical solutions

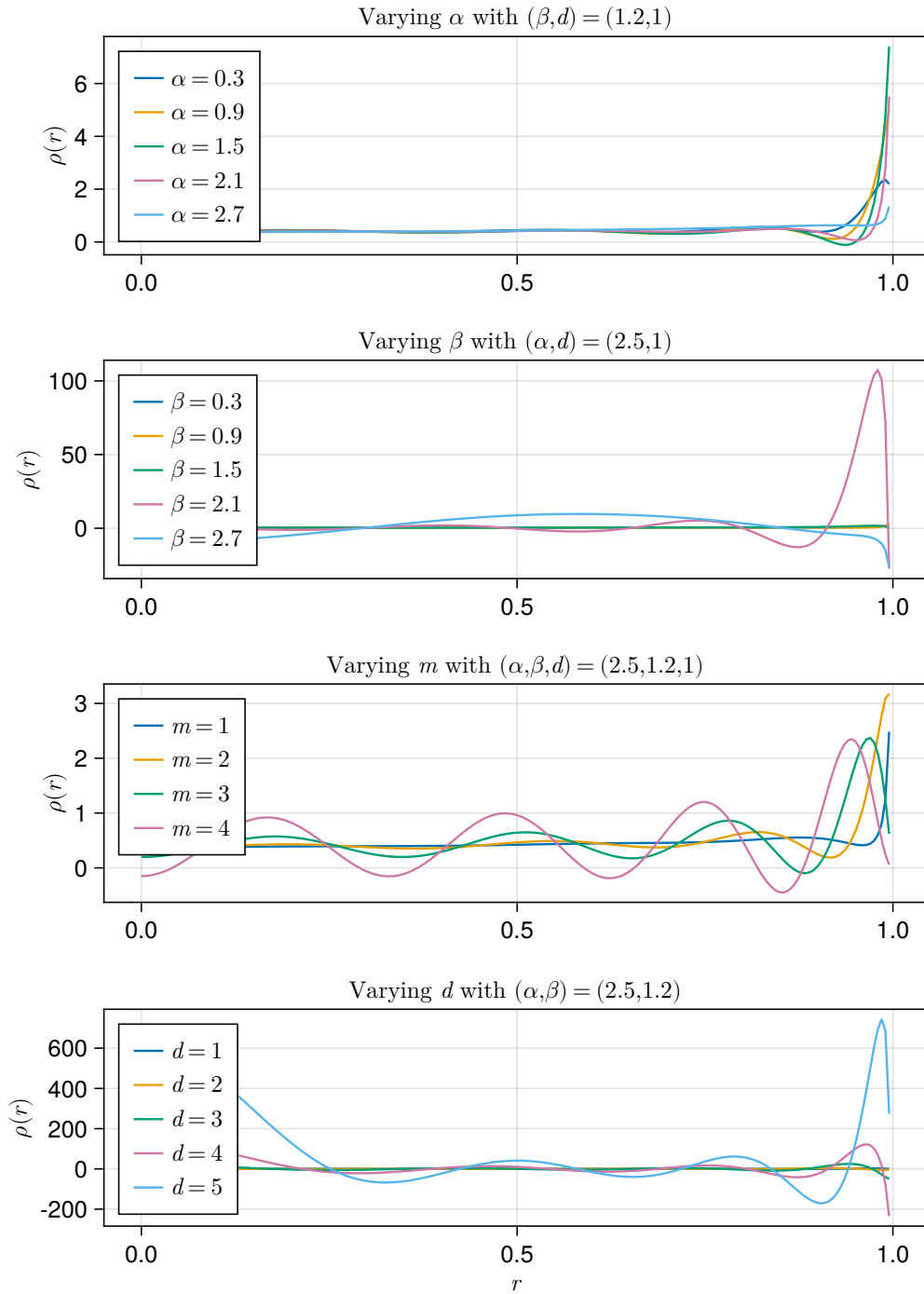
## 4.7 Discussion

- [ ] How does one look at this topic? We should have [[Spectral Convergence]], hopefully.

**Figure 4.7:** Convergence to analytic solutions**Figure 4.8:** Convergence



**Figure 4.9:** Spatial energy dependence on  $r$

**Figure 4.10:** Varying parameters in the solver



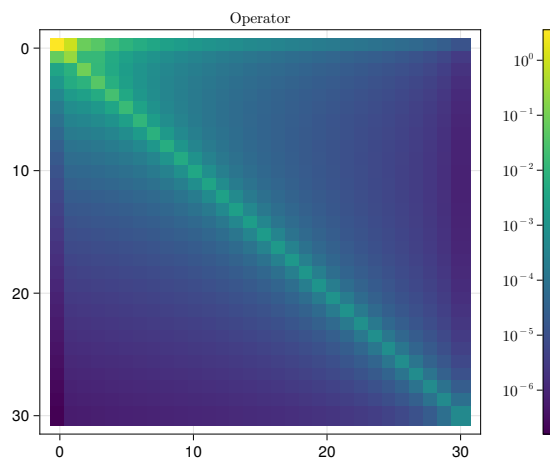
# Chapter 5

## General Kernel Spectral Method

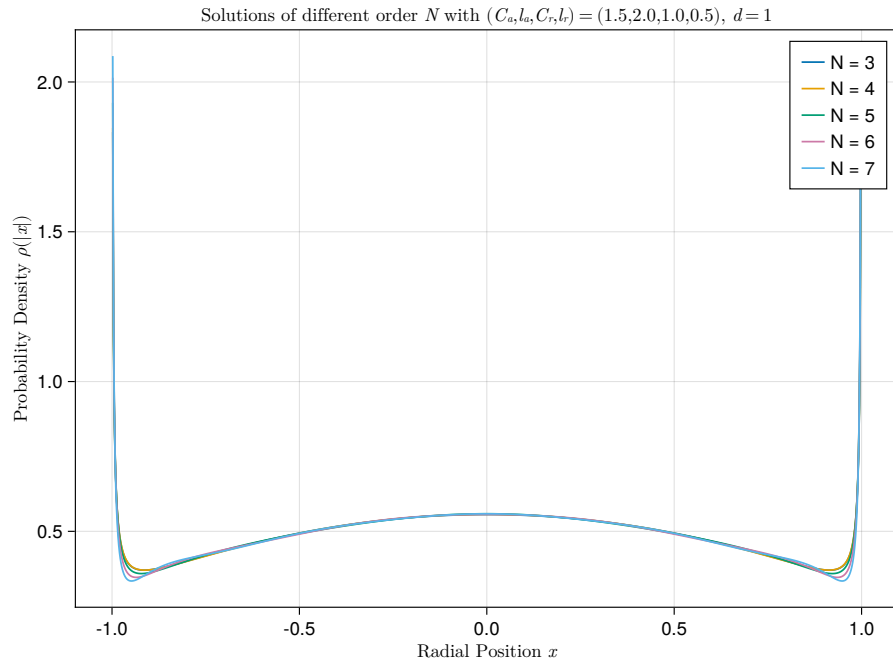
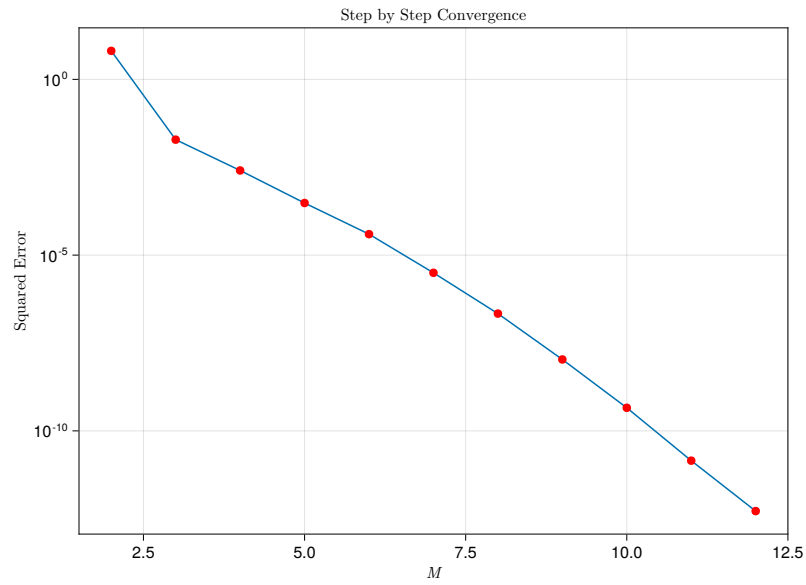
is a [[Spectral Method]] involving an [[Integral Equation]].

### 5.0.1 Structure

- Was ist ein General Kernel?
- How can we expand?
- Mehr Results als im vorigen Chapter [[Spectral Method]]



**Figure 5.1:** Operator

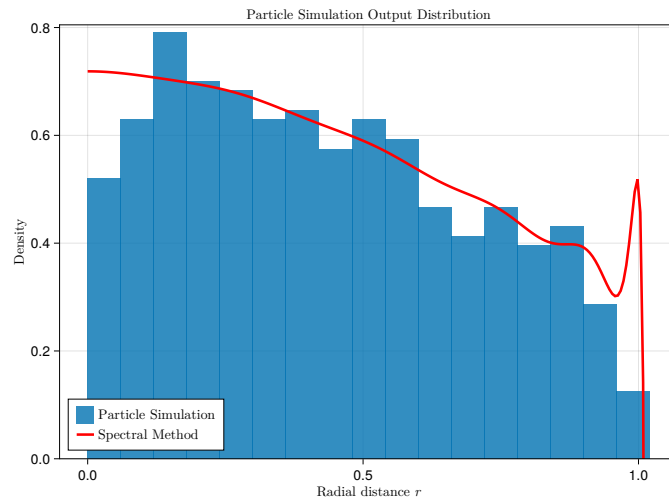
**Figure 5.2:** Solutions of increasing orders**Figure 5.3:** Convergence

# Chapter 6

## Implementation and Results

### 6.0.1 Structure

- Talk about Julia, C++ and the [[C++ Particle Integrator with GUI]]
- Numerical Results
  - Operator plots
  - Plots of Particle Densities
  - Difference between [[Spectral Method]] and [[Particle Simulator]] results



**Figure 6.1:** Comparison of the radial distance histogram from the simulation output with the solvers equilibrium measure  $\rho$ .

# Chapter 7

## Conclusion

In the present thesis, we explored the interesting realm of particle-particle interactions. Next to the written part, the reader will find an implementation of the particle simulator, including a Graphical User Interface (GUI), as well as the numerical solver.

Other approaches, such as the one in [Wu et al. 2015](#) show that ...

# Acronyms, Definitions and Theorems

GUI Graphical User Interface

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**Lemmata**

**Remarks**

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