

# Abstract

To be written.

This MMSC thesis will further explore general kernel spectral methods for finding equilibrium measures where initial progress made in [Gutleb, Carrillo and S. Olver 2020](#) and [Gutleb, Carrillo and S. Olver 2021](#).

**Keywords:** Equilibrium Measures

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

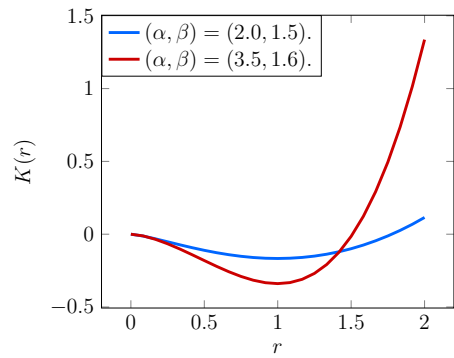
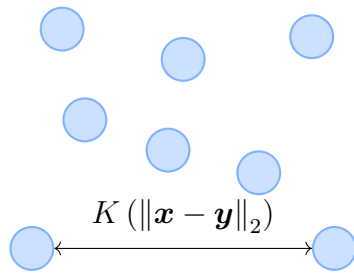
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# Chapter 1

## Introduction



**(a)**  $N = 8$  particles interacting with one another **(b)** Plot of attractive-repulsive potential functions through the potential  $K(r)$ .  
 $K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$  for different  $\alpha, \beta$ .

Cf. Figure 1.1a and Figure 1.1b.

All 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:

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

### 1.0.1 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

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### 2.0.1 aliases: Molecular Dynamics

Some input from the Wolfson Particle Physicist: 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).

### 2.0.2 Structure

- Definition: N-Body System (set of particles with position and velocity)
- Inertia / kinetic energy
- [[Potential]]s motivating a force  $F = -\nabla U$
- Write differential equation of movement  $\frac{dx_i}{dt}$
- Link to [[Particle Simulator]], give a Screenshot
- Introduce [[Continuous Limit]], write about particle density  $\rho(x)$
- [[Friction Term]] -> Energy Dissipation -> Different Plot

# Chapter 3

## Particle Simulator

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### 3.0.1 aliases: N-Body Simulator, Molecular Dynamics Simulator

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

### 3.0.2 Structure

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

### 3.0.3 Available Methods:

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



### 3.0.4 Available Solvers:

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

### 3.0.5 Implementations in [[My Dissertation]]:

- [[C++ Particle Integrator with GUI]]

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



**Figure 3.1:** Screenshot of the GUI

# 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

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

Todo: - [ ] is it alpha or beta in the exponent of  $(1-y^2)$ ?

### 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]].

One can even determine an explicit relationship between the coefficients in the Jacobi expansion by considering the [[Jacobi Matrix]].

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

$$\hat{Q}^\beta(x) = \sum_{k=1}^N \rho_k \int \|x - y\|^\beta (1 - \|y\|^2)^a P_k^{(a,b)}(2\|y\|^2 - 1) dy$$

### 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

$$L := \{f : \mathbb{R} \mapsto \mathbb{R} \mid f \text{ square integrable?}\}$$

**4.2.6 Definition: Gaussian Hypergeometric Function**

Written as

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

**4.2.7 Definition: Gegenbauer Polynomials****4.2.1 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

#### 4.2.2 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

Are given by

$$J_n^{(a,b)}(x) = \text{prefactor} \cdot {}_2F_1(\dots)$$

So are defined using the Gaussian Hypergeometric Function (cf. Definition 4.2.6).

#### 4.2.3 Nice Spectral Properties

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

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.

#### 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****4.2.4 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]]  $Q^\beta$ , acting on the coefficients  $\rho$ .

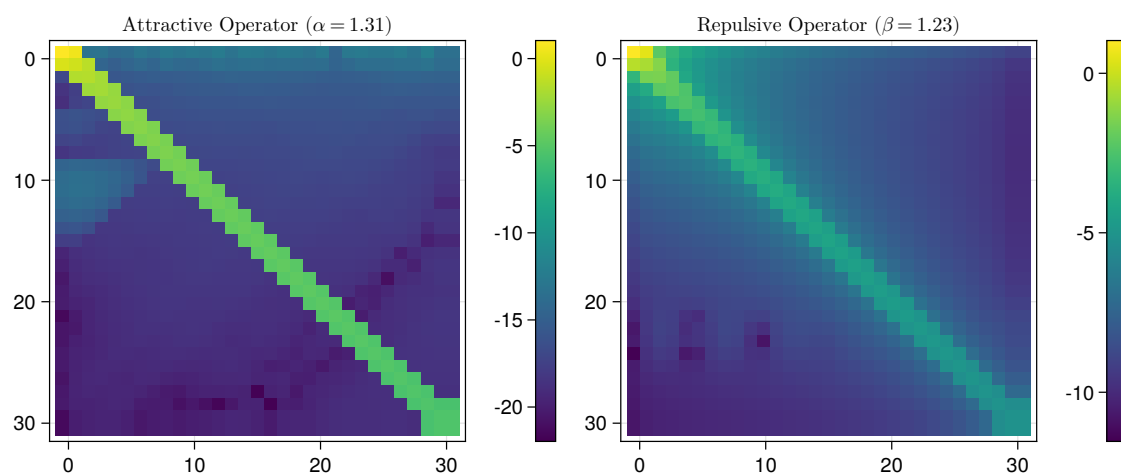
## 4.3 Derivation of Operator

Based on the [[Three-Term Recurrence Relationship]].

One can even determine an explicit relationship between the coefficients in the Jacobi expansion by considering the [[Jacobi Matrix]].

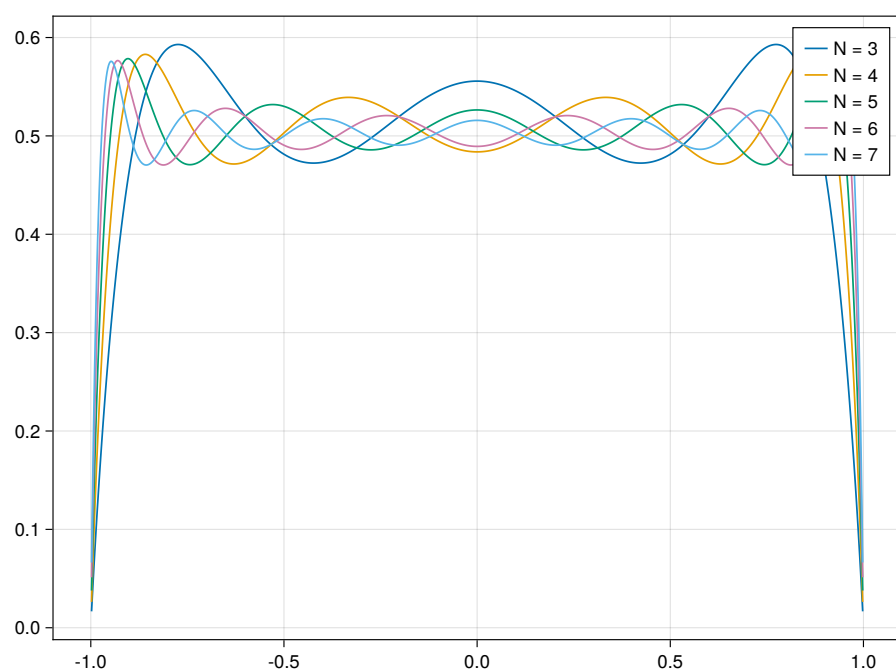
Considering the operator  $\hat{Q}^\beta[\rho]$  as in Theorem 4.2.1, from the [[Ansatz]]  $\rho(x)$  we have

$$\hat{Q}^\beta(x) = \sum_{k=1}^N \rho_k \int \|x - y\|^\beta (1 - \|y\|^2)^a P_k^{(a,b)}(2\|y\|^2 - 1) dy$$



**Figure 4.1:** The attractive and repulsive operators

## 4.4 Results



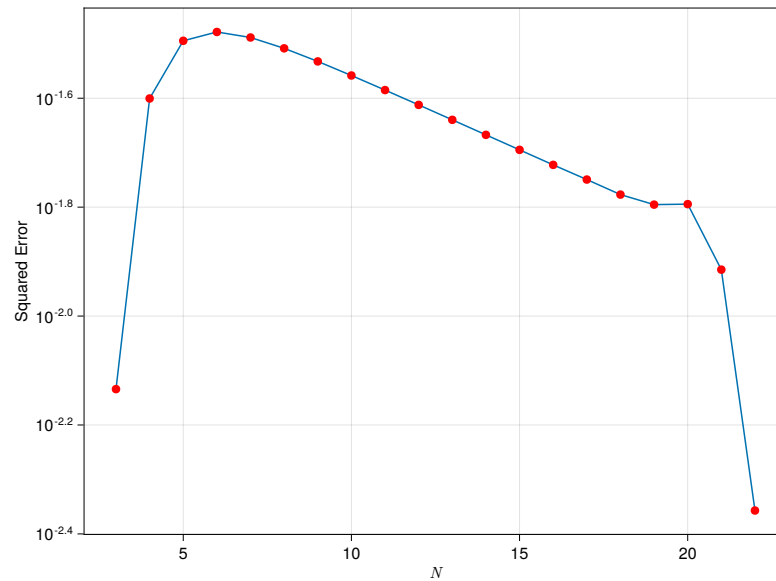
**Figure 4.2:** Solutions of increasing orders



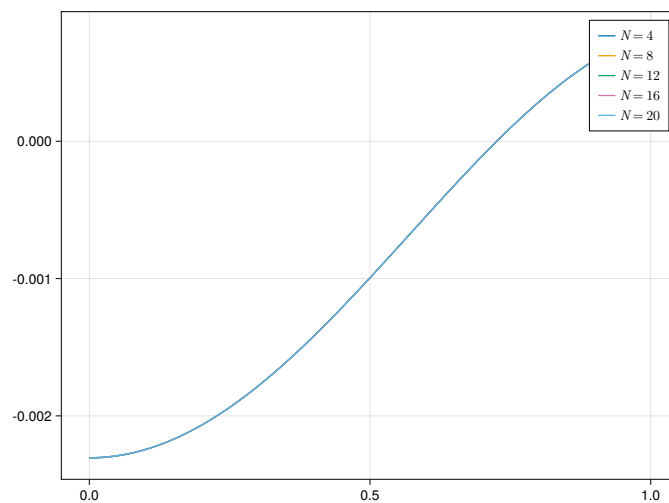
## 4.5 Discussion

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

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



**Figure 4.3:** Convergence



**Figure 4.4:** Spatial energy dependence on  $r$

# 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]]

# 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

# 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.

# Acronyms, Definitions and Theorems

GUI Graphical User Interface

20

## Definitions

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**Lemmata**

**Remarks**

# Bibliography

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## Appendix A – Supplemental Proofs