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

Contents

Chapter 1

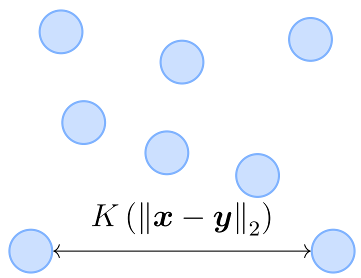
Introduction

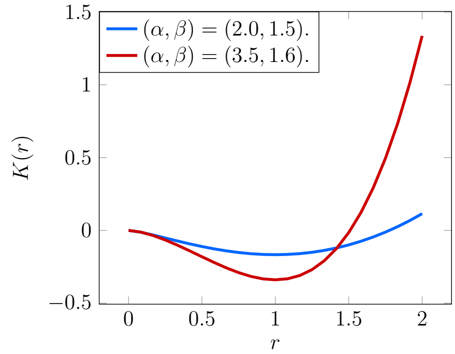
Let $\mathbb{N}$ denote the natural numbers (positive integers) without 0 and let $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. In the following, we will use **bold** notation for vectors, matrices will generally be denoted by a capital letter and scalars by a lowercase letter. We will frequently make use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

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 $B_1(\boldsymbol{x}) := \{\boldsymbol{y} \in \mathbb{R}^d \mid \|\boldsymbol{x} - \boldsymbol{y}\| \leq 1\}$ centered at the origin $\boldsymbol{x} = \mathbf{0}$. These volume integrals (often ended by $\mathrm{d}^d y$ or $\mathrm{d}V$) over the d-dimensional unit ball shall be written as

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

Note that some definitions of $B_1(\boldsymbol{x})$ are open sets, leaving out the shell $\{\boldsymbol{y} \in \mathbb{R}^d \mid \|\boldsymbol{x} - \boldsymbol{y}\| = 1\}$. 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.





(a) $N = 8$ particles interacting with one another through the potential $K(r)$.

(b) Plot of attractive-repulsive potential functions $K(r) = \frac{r^\alpha}{\alpha} - \frac{r^\beta}{\beta}$ for different α, β.

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

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

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!)

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

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:

$$xC_n^{(\lambda)}(x) = \tfrac{(n+2\lambda-1)}{2(n+\lambda)}C_{n-1}^{(\lambda)}(x) + \tfrac{n+1}{2(n+\lambda)}C_{n+1}^{(\lambda)}(x). \tag{1.1}$$

1.0.1 Theorem: Two term recurrence of Q^α

The integral operator

$$Q^\alpha\left[u\right](x) = \int_{-1}^{1} |x-y|^\alpha u(y)\,\mathrm{d}y$$

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

$$xQ^\alpha\left[wC_n^{(\lambda)}\right](x) = \kappa_1 Q^\alpha\left[wC_{n-1}^{(\lambda)}\right](x) + \kappa_2 Q^\alpha\left[wC_{n+1}^{(\lambda)}\right](x),$$

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

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

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?

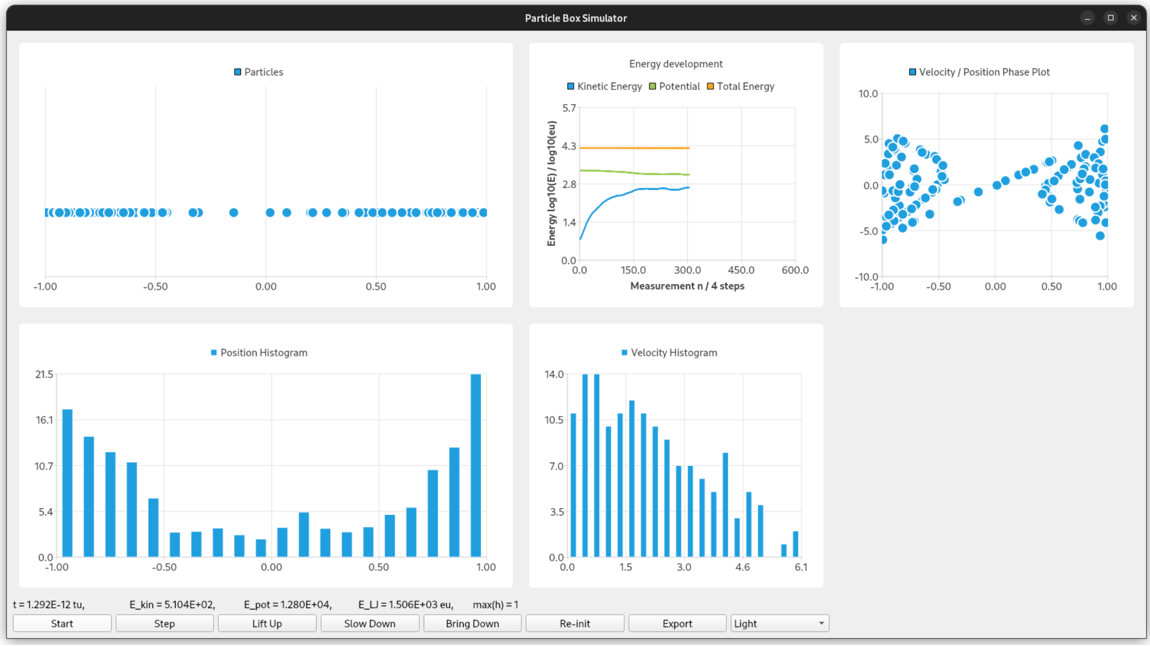


Figure 3.1: Screenshot of the GUI

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

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

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 $\rho(\boldsymbol{x})$ (cf. Definition 4.2.1) we have

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

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

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

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

Are given by

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

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

4.2.1 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

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

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

4.2.14 Definition: Rising Factorial

4.2.2 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 φ_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 $p = 1, 2, \ldots$ so $p \in \mathbb{N}$.
Source: 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:

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

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:

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

which is used to construct the [[Spectral Method]] [[Operator]] Q^β, acting on the coefficients $\boldsymbol{\rho}$.

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 $\rho(\boldsymbol{x})$ (cf. Definition 4.2.1) we have

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

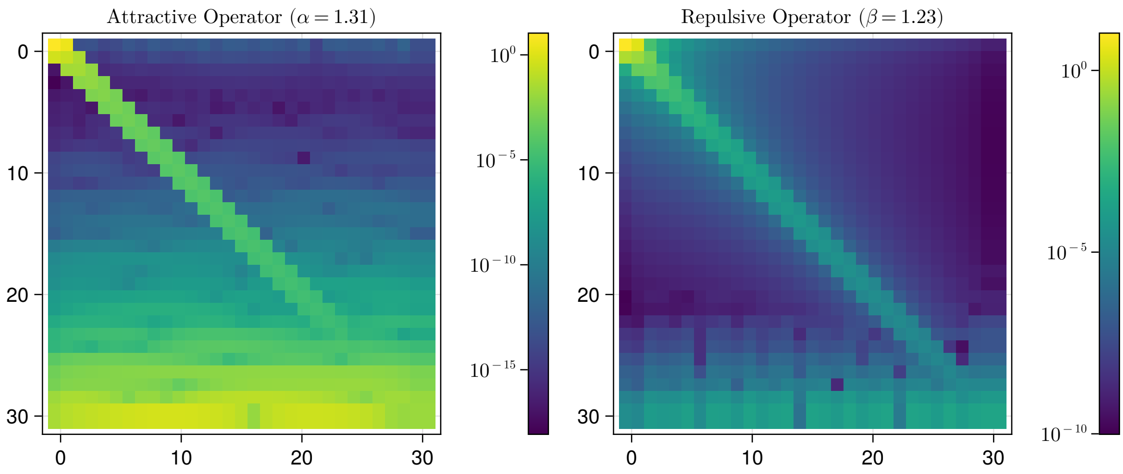


Figure 4.1: The attractive and repulsive operators (matrices), values are in log10-scale.

4.4 Results

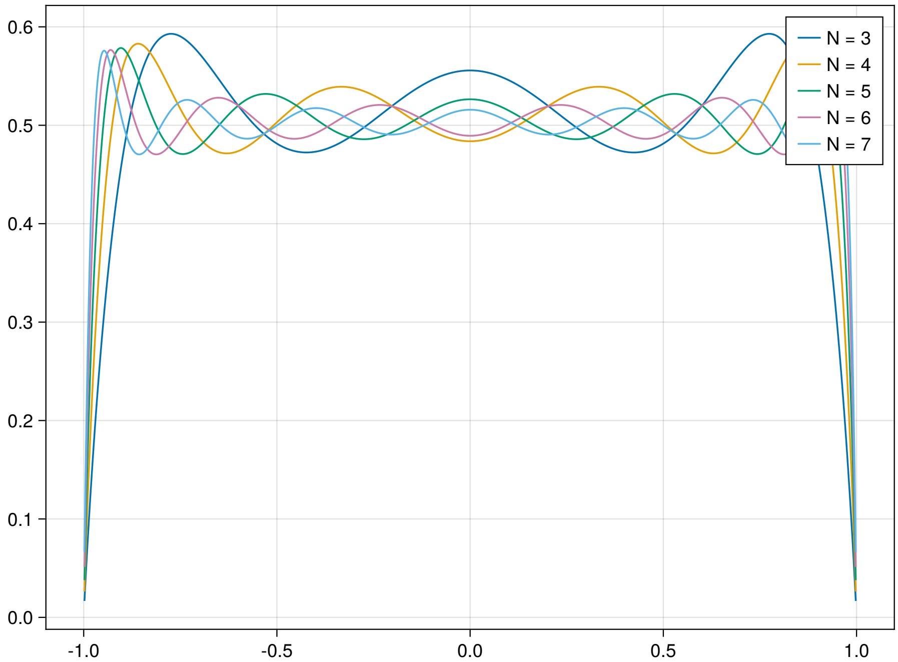


Figure 4.2: Solutions of increasing orders

4.5 Outer Optimisation Routine

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

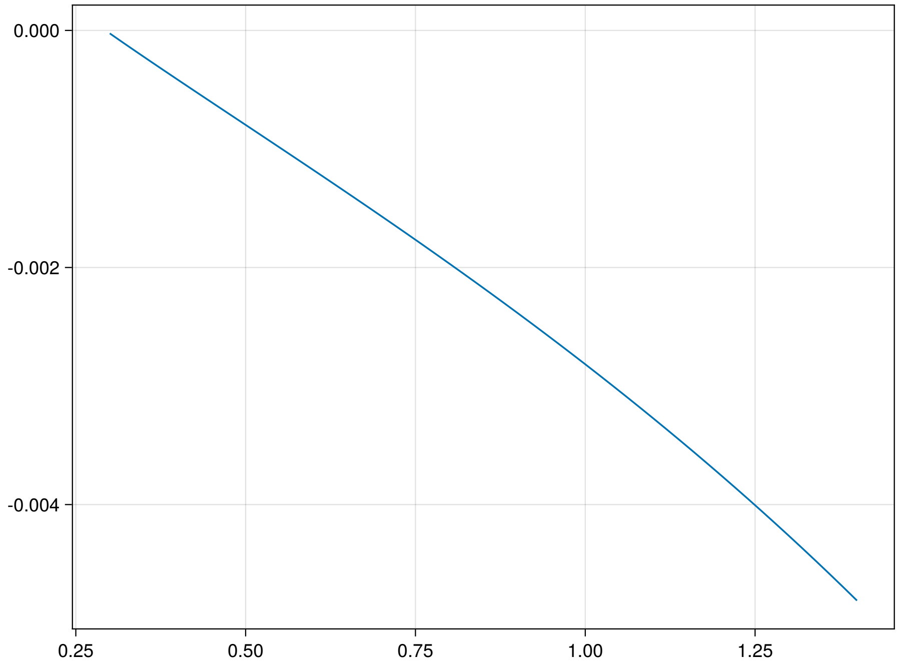


Figure 4.3: Outer Optimisation

4.6 Discussion

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

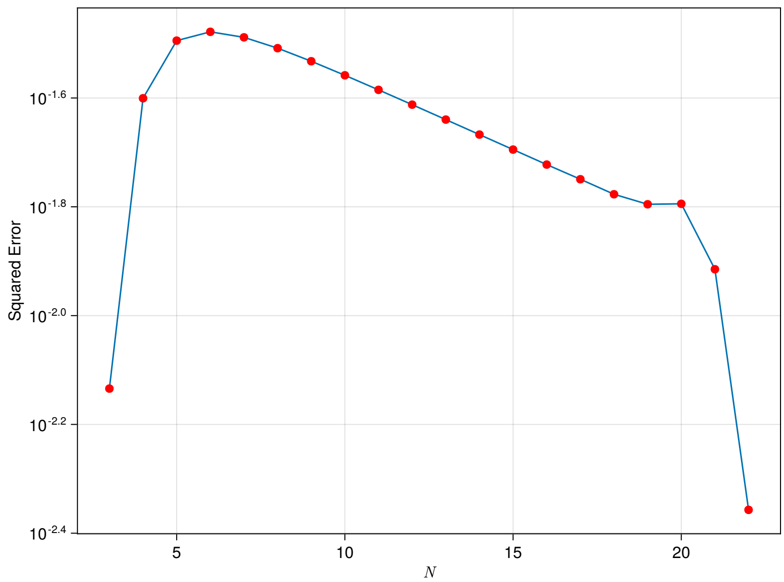


Figure 4.4: Convergence

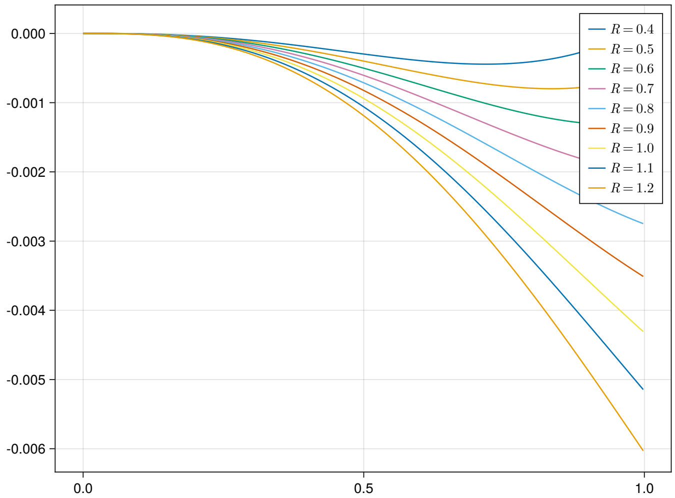


Figure 4.5: Spatial energy dependence on r

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 22

Definitions

Theorems

Lemmata

Remarks

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Appendix A – Supplemental Proofs