



**FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA**

Discretization of the Dirac-operator for fermions
within magnetic field

Theoretisch-Physikalisches Institut
Physikalisch-Astronomische Fakultät
Friedrich-Schiller-Universität Jena

Bachelorarbeit

zur Erlangung des akademischen Grades
Bachelor of Science

Vladislav Guschakowski
geboren am 25.11.1998 in Almaty

Erstprüfer: Prof. Dr. Andreas Wipf

Zweitprüfer: Dr. Michael Mandl

Abgabedatum: 24.03.2024

Table of Contents

Introduction	3
1. Theoretical foundations	4
1.1. Quantum Field Theories	4
1.2. Quantization of the magnetic field	5
2. Eigenmodes and Dirac operator	8
2.1. Zero modes of the eigenfunctions	9
2.2. Raising and lowering operators	12
2.3. Zeroes of the zero modes	16
2.4. Eigenfunctions of the Dirac operator	17
3. Discretization of the Dirac operator	19
3.1. Spectral resolution	19
3.2. Simplifying the spectral sum	22
3.3. Alternative representations of the first matrix element	25
3.4. Quadrature tests	27
3.5. Discretizing Space	29
Conclusion	32
A. Appendix	33
A.1. Hermite polynomials	33
A.2. Quadrature	34
A.3. Normalization checks	36
A.4. Jacobi theta function	36
A.5. Verification of the zeroes of the zero modes via residue theorem	37
A.6. Verification of the first matrix element after application of Christoffel-Darboux	40
Bibliography	42
Eidesstattliche Erklärung	44

Introduction

In the realm of physics, particularly within the intricate framework of quantum field theory, the discretization of operators stands as a foundational method of paramount importance. Because of the complications of many physical problems, it is often necessary to use numerical methods to find answers to many questions. To be able to apply those methods, one first needs to find discrete versions of normally continuous mathematical objects. Of special interest in quantum field theory is the discretization of the Dirac operator.

In statistical quantum field theory, this operator can be used to determine the thermodynamical state of equilibrium of a fermionic particle constellation. An especially interesting phenomenon is the one of inhomogeneous ground states of equilibrium. If the considered theory is invariant under translations, one might expect for a state of equilibrium that physical properties become the same everywhere, similar to differences in temperature dissolving over time. But this is not always the case. Former study shows, that for interacting fermions in 1+1 dimensions inhomogeneous phases do exist. Also, in 2+1 dimensions an inhomogeneous state of equilibrium might be possible, but the effect did not prove to be strong enough to be distinguishable from numerical noise. Theoretically, a magnetic field could increase these effects and hopefully make them visible. [1] [2]

To achieve this, the discretization of the Dirac operator of fermions within an magnetic field is a logical first step. In lattice field theory there are already many different approaches in to this in the literature, for example Wilson- [3], KS- [3], overlap- [4] or domain-wall-fermions [5]. All attempt to avoid the so called doubling problem [6] of a naive discretization of just using a completely equidistant grid. This thesis will provide an attempt to find a new discretization. For this, we will attempt to discretize the continuous solutions of the eigenvalue equation of the Dirac operator by application of a fitting discretization method. Depending on the type of the solution, spectral or pseudo-spectral methods are useful tools for this operation. Those methods basically apply an expansion in a certain basis, similar to a Fourier series. The Fourier series is in fact one of the spectral methods, which works well as long as the functions of interest are periodic. If that is not the case, it is better to apply a pseudo-spectral method, like the Gaussian quadrature. [7] [8]

This thesis presents an attempt to find a discretization of the Dirac operator for fermions in 2+1 dimensions within a square (in the space dimensions) and a constant magnetic field. After presenting a few theoretical foundations, the second chapter is dedicated to solving the eigenvalue equation of the Dirac operator. For this, the identification of ladder operators proves to be quite useful. On a side note, the determination of the zeroes of the zero modes will also be presented. Finally, chapter three is dedicated to the study of the discretization. The time and one space dimension will be discretized, while the second space dimension proves to be more challenging. The discretization of this third dimension could not be achieved as part of this thesis. Still, chapter three includes the study of the application of the Gaussian quadrature, which could lead to a discretization in the future.

1. Theoretical foundations

1.1. Quantum Field Theories

The sources of the present chapter are [1] and [9].

A *Quantum Field Theory* is the best way modern physics can model elementary particles. The main idea is to introduce fields $\psi(t, \vec{x})$, where particles are given by excitations of those fields. Analogously to Lagrangian mechanics the action S is given by the time-integral over the Lagrange-function L . But since we are now dealing with fields, the *Lagrange-function* itself is given by a space-integral over a *Lagrange-density* $\mathcal{L}(\psi, \partial_\mu\psi)$ (Lagrangian). So, overall the action is given by a spacetime-integral

$$S(\psi) = \int \mathcal{L}(\psi, \partial_\mu\psi) \, d^d x .$$

Also completely analogous to classical mechanics, the time and space evolution of these fields is given by calculus of variations, which leads to the *Euler-Lagrange-equations*

$$\frac{\partial \mathcal{L}}{\partial \psi} = \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi)} .$$

The physical predictions are given by expectation values of observables \mathcal{O} , similar to quantum mechanics. In the language of the *path integral formulation* they are given by a weighted sum over all possible field configurations

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O}(\psi) e^{iS(\psi)} \mathcal{D}\psi ,$$

where Z is a normalization factor. When applying the so-called *Wick-rotation*, consisting of a transformation of the time variable $t \rightarrow i\tau$ and the corresponding analytic continuation to imaginary times, Z can be expressed in terms of the *Euclidean action* S_E

$$Z = \int e^{-S_E(\psi)} \mathcal{D}\psi .$$

Writing Z this way allows to draw a powerful connection. When considering the special case of a closed path over an imaginary time interval $\Delta\tau \equiv \beta$, this Euclidean action takes the form of a classical Hamiltonian

$$Z = \text{tr} \left(e^{-\beta \hat{H}} \right) .$$

Now the normalization factor is just the *canonical partition function*. This way, results from computations on the Lagrangian lead to thermodynamical predictions. Especially of interest is the so called *Dirac operator* \mathcal{D} , which governs fermionic quantum field theories. In particular, most relevant fermionic theories are of the form

$$\mathcal{L} = \bar{\psi} \mathcal{D} \psi$$

or can be brought into that form via a suitable *Hubbard-Stratonovich-transformation*. Here, ψ denotes an N_f -tuple of fermion fields, N_f being the number of fermionic flavors, which we assume to be mass-degenerate. Within the so called *t'Hooft-limit* of infinitely many flavors, *stationary phase approximation* allows to determine the state of equilibrium via a minimization problem containing the

Dirac operator. That is the reason, why this work will study the Dirac operator of such a Lagrangian in order to allow the determination of the state of equilibrium for a given physical situation.

More specifically, we are interested in fermions within an external magnetic field, which is why the Lagrangian of interest is given by

$$\mathcal{L} = \bar{\psi} i \underbrace{\gamma^\mu D_\mu}_{=\mathcal{D}} \psi + im\bar{\psi}\psi .$$

Here, i is the imaginary unit, γ^μ are the Dirac matrices, $D_\mu := \partial_\mu - iA_\mu$ is the covariant derivative with the gauge field A_μ and m is the fermionic mass.

1.2. Quantization of the magnetic field

The sources of the present chapter are [2] and [10].

During this work we will be considering fermions within a square plane with length L , while a constant magnetic field B passes orthogonally through the area. We normally wish to impose periodic boundary conditions in both x - and y -directions. But when considering the magnetic flux through the plane L^2 we find

$$\begin{aligned} BL^2 &= \iint_V B \, dx dy \\ &= \iint_V (\partial_x A_y - \partial_y A_x) \, dx dy \\ &= \int_0^L [A_y(x=L, y) - A_y(x=0, y)] \, dy - \int_0^L [A_x(x, y=L) - A_x(x, y=0)] \, dx \end{aligned} \quad (1)$$

where it becomes obvious that periodic boundary conditions for the gauge field A_μ would imply a trivial magnetic field $B = 0$ (since (1) would vanish). But what we can do is make use of the gauge invariance of the theory

$$A_\mu \longrightarrow A_\mu + \partial_\mu \Lambda$$

where Λ can be chosen as any arbitrary smooth function. The gauge transformation for the operator equation is

$$\begin{aligned} \mathcal{D} &\longrightarrow \gamma^\mu (\partial_\mu - iA_\mu - i\partial_\mu \Lambda) = e^{i\Lambda} \gamma^\mu (\partial_\mu - iA_\mu) e^{-i\Lambda} \\ &= e^{i\Lambda} \mathcal{D} e^{-i\Lambda} . \end{aligned}$$

From this we directly find the gauge transformation of the eigenfunctions

$$\begin{aligned} i\mathcal{D}\psi = \lambda\psi &\longrightarrow e^{i\Lambda} i\mathcal{D}e^{-i\Lambda}\psi' = \lambda\psi' \\ &\iff \psi' = e^{i\Lambda}\psi . \end{aligned}$$

Now we can consider the gauge transformation of

$$A_\mu(x+L, y) - A_\mu(x, y) \longrightarrow A_\mu(x+L, y) + \partial_\mu \Lambda(x+L, y) - A_\mu(x, y) - \partial_\mu \Lambda(x, y)$$

and choose a gauge such that

$$\begin{aligned} A_\mu(x+L, y) + \partial_\mu \Lambda(x+L, y) - A_\mu(x, y) - \partial_\mu \Lambda(x, y) &\stackrel{!}{=} 0 \\ \iff A_\mu(x+L, y) - A_\mu(x, y) &= \underbrace{\partial_\mu [\Lambda(x, y) - \Lambda(x+L, y)]}_{\equiv \Lambda^{(1)}(x, y)}. \end{aligned} \quad (2)$$

Analogously we get for the y -direction

$$A_\mu(x, y+L) - A_\mu(x, y) = \partial_\mu \Lambda^{(2)}(x, y). \quad (3)$$

These two conditions imply, that the gauge field is periodic up to a gauge transformation in both x - and y -directions. This means, that the same is true for the spinor field

$$\psi(x+L, y) = e^{i\Lambda^{(1)}(x, y)} \psi(x, y) \quad \text{and} \quad \psi(x, y+L) = e^{i\Lambda^{(2)}(x, y)} \psi(x, y). \quad (4)$$

If we now use (2) and (3) in (1) we find

$$\begin{aligned} BL^2 &= \int_0^L [A_y(x=L, y) - A_y(x=0, y)] dy - \int_0^L [A_x(x, y=L) - A_x(x, y=0)] dx \\ &= \int_0^L \partial_y \Lambda^{(1)}(0, y) dy - \int_0^L \partial_x \Lambda^{(2)}(x, 0) dx \\ &= \Lambda^{(1)}(0, L) - \Lambda^{(1)}(0, 0) - \Lambda^{(2)}(L, 0) + \Lambda^{(2)}(0, 0). \end{aligned} \quad (5)$$

For consistency reasons we have to make sure, that two independent gauge transformations for the x - and y -directions commute with each other

$$\begin{aligned} \psi(x+L, y+L) &= \psi(x+L, y+L) \\ \iff e^{i\Lambda^{(1)}(x, y+L)} \psi(x, y+L) &= e^{i\Lambda^{(2)}(x+L, y)} \psi(x+L, y) \\ \iff e^{i[\Lambda^{(1)}(x, y+L) + \Lambda^{(2)}(x, y)]} \psi(x, y) &= e^{i[\Lambda^{(2)}(x+L, y) + \Lambda^{(1)}(x, y)]} \psi(x, y). \end{aligned}$$

Since the phases are periodic, we find

$$\Lambda^{(1)}(x, y+L) + \Lambda^{(2)}(x, y) - \Lambda^{(2)}(x+L, y) - \Lambda^{(1)}(x, y) = \nu 2\pi$$

where $\nu \in \mathbb{Z}$. If we now choose explicitly $x = y = 0$ we can make use of (5)

$$\begin{aligned} \Lambda^{(1)}(0, L) + \Lambda^{(2)}(0, 0) - \Lambda^{(2)}(L, 0) - \Lambda^{(1)}(0, 0) &= \nu 2\pi \\ \iff BL^2 &= \nu 2\pi \\ \iff B &= \frac{\nu 2\pi}{L^2} \end{aligned} \quad (6)$$

to find that the magnetic field through a finite surface L^2 must be quantized. ν is called the *instanton number* and is thus a quantum number describing the amount of magnetic flux quanta passing the surface. The smallest possible flux quantum is $B_{\min} = \frac{2\pi}{L^2}$.

Finally, there are two more mathematical tools, which need proper introduction. Those are *Hermitite polynomials* and the *Gaussian quadrature*. Many different introductions to those topics can be found, as for example in [8], [7] and [11].

Hermite polynomials are a set of orthogonal polynomials, which appear as the eigenfunctions of the quantum harmonical oscillator. They fulfill useful recursion relations and they define the *Hermite-Gauss weights*. These weights allow to substitute integrals of polynomials by finite sums via the Gaussian quadrature. A more detailed account on both those topics can be found in the appendices A.1 and A.2.

2. Eigenmodes and Dirac operator

The first aim of this work is finding the eigenmodes and -values of the Dirac operator in question. For this, we first construct the diagonalized squared operator. We then determine the eigenmodes and -values of this squared operator, where we are able to identify ladder operators. Those operators allow to compute any mode from the zero mode, which can be found in chapter 2.2. This is why we must determine the zero mode beforehand, which happens in chapter 2.1. When we know everything about the squared operator, we can construct the eigenmodes and -values of the original Dirac operator, as found in chapter 2.4. Furthermore, chapter 2.3 contains the determination of the zeroes of the zero modes.

As already mentioned in chapter 1.1, the Lagrangian we wish to study is

$$\mathcal{L} = \bar{\psi} \underbrace{i \gamma^\mu D_\mu}_{=:\not{D}} \psi + im \bar{\psi} \psi .$$

The specific constellation of interest is the same as in chapter 1.2. We want to study constant magnetic fields passing orthogonally through a square surface in the x - y -plane. There should not be any electric field, from which follows $A_0 = 0$. Thus, we wish to solve the eigenvalue equation of the Dirac operator

$$i\not{D}\psi = \lambda\psi \quad \text{with} \quad i\not{D} = i\gamma^0\partial_0 + i\gamma^i D_i$$

in 2+1 dimensions. Since this operator is the product of the imaginary unit i and a first order differential operator, it is hermitian and thus has real eigenvalues $\lambda \in \mathbb{R}$. In these dimensions we can choose a convenient representation for the *Dirac matrices* γ^μ by using the *Pauli matrices* σ_μ

$$\gamma^1 = \sigma_1, \quad \gamma^2 = \sigma_2, \quad \gamma^0 = \sigma_3$$

where one can check that this representation fulfills the defining property of the Dirac matrices

$$\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu} \sigma_0 .$$

In the chosen representation we find explicitly

$$i\not{D} = \begin{pmatrix} i\partial_0 & A^\dagger \\ A & -i\partial_0 \end{pmatrix} \quad (7)$$

with $A := i(D_1 + iD_2)$ and (since D_μ is a first order differential operator) $A^\dagger = i(D_1 - iD_2)$. From this operator we can construct a diagonal operator by studying its square

$$(i\not{D})^2 = \begin{pmatrix} -\partial_0^2 + A^\dagger A & 0 \\ 0 & -\partial_0^2 + AA^\dagger \end{pmatrix} \quad (8)$$

where we used, that the magnetic field should be constant in time $\partial_0 A_i = 0$. We did this, because it is much simpler to find the eigenfunctions and -values of a diagonal operator. From those, the eigenfunctions and values of the original operator can be easily constructed. Now we can separate this

matrix and identify the field strength tensor $F_{\mu\nu}$

$$\begin{aligned}
 (i\mathcal{D})^2 &= -\partial_0^2 \mathbb{1} - D_i^2 \mathbb{1} - \gamma^0 i \underbrace{[D_1, D_2]}_{=-i(\partial_1 A_2 - \partial_2 A_1)} \\
 &= -\partial_0^2 \mathbb{1} - D_i^2 \mathbb{1} - \gamma^0 \underbrace{F_{12}}_{=B} \\
 &= (-\partial_0^2 - D_i^2) \mathbb{1} - \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix} .
 \end{aligned}$$

Since both $A^\dagger A$ and AA^\dagger are time independent, they commute with ∂_0^2 . Explicitly they are

$$AA^\dagger = -D_i^2 + B \quad \text{and} \quad A^\dagger A = -D_i^2 - B . \quad (9)$$

We want to solve their corresponding eigenvalue equations, where we have non-negative eigenvalues (since they are both hermitian and we obtained them by squaring an operator)

$$A^\dagger A \varphi_n = \lambda_n^2 \varphi_n \quad \text{and} \quad AA^\dagger \chi_n = \lambda_n^2 \chi_n . \quad (10)$$

If we assume $B > 0$ we find from (9) that

$$AA^\dagger = A^\dagger A + 2B > A^\dagger A . \quad (11)$$

From this condition we find that there are only zero modes for $A^\dagger A$. So now we have constructed the squared Dirac operator (8) and go on to determine the eigenmodes of its diagonal elements.

2.1. Zero modes of the eigenfunctions

We have constructed the diagonalized squared Dirac operator (8) and now want to find its eigenmodes so that we can construct the eigenmodes of the original Dirac operator (7). Since ∂_0^2 commutes with both AA^\dagger and $A^\dagger A$, which were given by (9), the eigenfunctions of the squared operator are

$$\psi_1 = e^{i\omega t} \begin{pmatrix} \varphi \\ 0 \end{pmatrix} \quad \text{and} \quad \psi_2 = e^{i\omega t} \begin{pmatrix} 0 \\ \chi \end{pmatrix} . \quad (12)$$

So the zero modes of the squared operator are determined by the zero modes of the operators AA^\dagger and $A^\dagger A$, because of (10). We already know from (11) that we only have zero modes for $A^\dagger A$. So we search for eigenmodes φ such that

$$\begin{aligned}
 A^\dagger A \varphi &= 0 \\
 \implies (\varphi, A^\dagger A \varphi) &= 0 \\
 \iff (A \varphi, A \varphi) &= 0
 \end{aligned}$$

which is fulfilled by

$$A \varphi = 0 .$$

But since we obviously also have $A \varphi = 0 \implies A^\dagger A \varphi = 0$ we find

$$A^\dagger A \varphi = 0 \iff A \varphi = 0 .$$

So it is enough to only study the following differential equation

$$\begin{aligned} A\varphi &= 0 \\ \iff (iD_1 - D_2)\varphi &= 0 \\ \iff [A_x - \partial_y + i(\partial_x - A_y)]\varphi &= 0 . \end{aligned}$$

Now we can choose a gauge such that

$$A_x(y) = -By \quad \text{and} \quad A_y = 0$$

where one can check that this choice fulfills the necessary condition $F_{12} = B$. This leads to the simpler differential equation

$$[-By - \partial_y + i\partial_x]\varphi = 0 .$$

A product ansatz $\varphi(x, y) = X(x)Y(y)$ leads to the solutions

$$\varphi(x, y) = Ce^{i\alpha x} e^{-\frac{B}{2}\left(y + \frac{\alpha}{B}\right)^2} \quad (13)$$

with $C \in \mathbb{C}$ and $\alpha \in \mathbb{C}$. These are infinitely many solutions. But we must also fulfill the boundary conditions (4) in both x - and y -direction. So we must determine the gauge functions $\Lambda^{(1)}$ and $\Lambda^{(2)}$

$$\begin{aligned} A_x(y) &= -By \\ \iff A_x(y + L) &= -B(y + L) \\ \iff A_x(y) + \partial_x \Lambda^{(1)} &= A_x(y) - BL \\ \iff \Lambda^{(1)} &= -BLx + C_1 \end{aligned}$$

and analogously $\Lambda^{(2)} = C_2$. We choose $C_1 = 0 = C_2$. With this we obtain the explicit boundary conditions

$$\psi(x + L) = \psi(x) \quad \text{and} \quad \psi(y + L) = e^{-iBLx}\psi(y) . \quad (14)$$

Because of (12), the boundary conditions only apply to φ and χ . Let us apply the first one of the conditions (14) to the zero modes (13)

$$\begin{aligned} \varphi(x + L) &= \varphi(x) \\ \iff e^{i\alpha x + i\alpha L} &= e^{i\alpha x} \\ \iff \alpha &= \frac{2\pi}{L}p \equiv \alpha_p \end{aligned} \quad (15)$$

with $p \in \mathbb{Z}$. So the zero modes take on the new form

$$\varphi_p(x, y) = Ce^{i\alpha_p x} e^{-\frac{B}{2}\left(y + \frac{\alpha_p}{B}\right)^2} , \quad p \in \mathbb{Z} . \quad (16)$$

Let us now apply the second condition of (14) with $k \in \mathbb{Z}$

$$\begin{aligned} \varphi_p(y + kL) &= e^{-iBkLx}\varphi_p(y) \\ \iff \underbrace{e^{i\alpha_p x}}_{\text{phase}} \underbrace{e^{-\frac{B}{2}\left(y + kL + \frac{\alpha_p}{B}\right)^2}}_{\text{value}} &= \underbrace{e^{i(\alpha_p - BkL)x}}_{\text{phase}} \underbrace{e^{-\frac{B}{2}\left(y + \frac{\alpha_p}{B}\right)^2}}_{\text{value}} . \end{aligned}$$

Since the values must be equal, we find in the exponent that for all k we have to identify $\frac{\alpha_p}{B} + kL$ as the same solution. This is just a modulo $\alpha_p + BL\mathbb{Z}$, which leaves only $0 \leq \alpha_p < BL$ as different solutions. So when we use the explicit forms of α_p (15) and the magnetic field B (6) we find that

$$\begin{aligned} 0 &\leq \alpha_p < BL \\ \iff 0 &\leq \frac{2\pi}{L}p < \frac{\nu 2\pi}{L^2}L \\ \iff 0 &\leq p < \nu \end{aligned}$$

which leaves exactly ν zero modes. Their amount is thus given by the instanton number. So we have to consider a superposition of all identified solutions as one single eigenmode

$$\varphi_{0,p}(x, y) = C \sum_{k \in \mathbb{Z}} e^{i(\alpha_p + kBL)x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2}, \quad 0 \leq p < \nu. \quad (17)$$

The next task is to normalize them. For that we study

$$\langle \varphi_{0,p} | \varphi_{0,p'} \rangle = \int_0^L \int_0^L |C|^2 \sum_{k, k' \in \mathbb{Z}} e^{-i(\alpha_p + kBL)x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2} e^{i(\alpha_{p'} + k'BL)x} e^{-\frac{B}{2}(y + \frac{\alpha_{p'}}{B} + k'L)^2} dx dy.$$

Let us first consider the x -dependent part of the integral

$$\begin{aligned} e^{-i(\alpha_p + kBL)x} e^{i(\alpha_{p'} + k'BL)x} &= e^{i[\alpha_{p'} - \alpha_p + BL(k' - k)]x} \\ &\stackrel{(15)}{=} e^{i[\frac{2\pi}{L}p' - \frac{2\pi}{L}p + BL(k' - k)]x} \\ &\stackrel{(6)}{=} e^{i\frac{2\pi}{L}[p' - p + \nu(k' - k)]x}. \end{aligned}$$

Since $0 \leq p, p' < \nu$, the exponent consists of the sum a multiple of ν and a $p' - p$, which is smaller than ν . When also considering, that the integral goes from 0 to L , integral of the phase above thus vanishes for any $p \neq p'$ or $k \neq k'$. At the same time the phase is 1 for $p = p'$ and $k = k'$. So we find for the scalar product

$$\begin{aligned} \langle \varphi_{0,p} | \varphi_{0,p'} \rangle &= |C|^2 L \delta_{p,p'} \int_0^L \sum_{k, k' \in \mathbb{Z}} \delta_{k,k'} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2} e^{-\frac{B}{2}(y + \frac{\alpha_{p'}}{B} + k'L)^2} dy \\ &= |C|^2 L \delta_{p,p'} \sum_{k \in \mathbb{Z}} \int_0^L e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2} e^{-\frac{B}{2}(y + \frac{\alpha_{p'}}{B} + kL)^2} dy. \end{aligned}$$

We want to normalize the case $p = p'$ and solve the ensuing *Gaussian integral*. We find that

$$\begin{aligned} \langle \varphi_{0,p} | \varphi_{0,p} \rangle &= |C|^2 L \sum_{k \in \mathbb{Z}} \int_0^L e^{-B(y + \frac{\alpha_p}{B} + kL)^2} dy \\ &= |C|^2 L \int_{\mathbb{R}} e^{-B(y + \frac{\alpha_p}{B})^2} dy \\ &= |C|^2 L \sqrt{\frac{\pi}{B}} \stackrel{!}{=} 1 \end{aligned} \quad (18)$$

which gives for the normalization constant

$$C = e^{i\varphi} \sqrt[4]{\frac{B}{\pi L^2}}$$

where we can choose $\varphi = 0$. So the normalized zero modes look like this

Zero modes of the operator $A^\dagger A$ (9)

$$\varphi_{0,p}(x, y) = \sqrt[4]{\frac{B}{\pi L^2}} \sum_{k \in \mathbb{Z}} e^{i(\alpha_p + kBL)x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2}, \quad 0 \leq p < \nu. \quad (19)$$

Plots of a few selected zero modes can be found in figure 1.

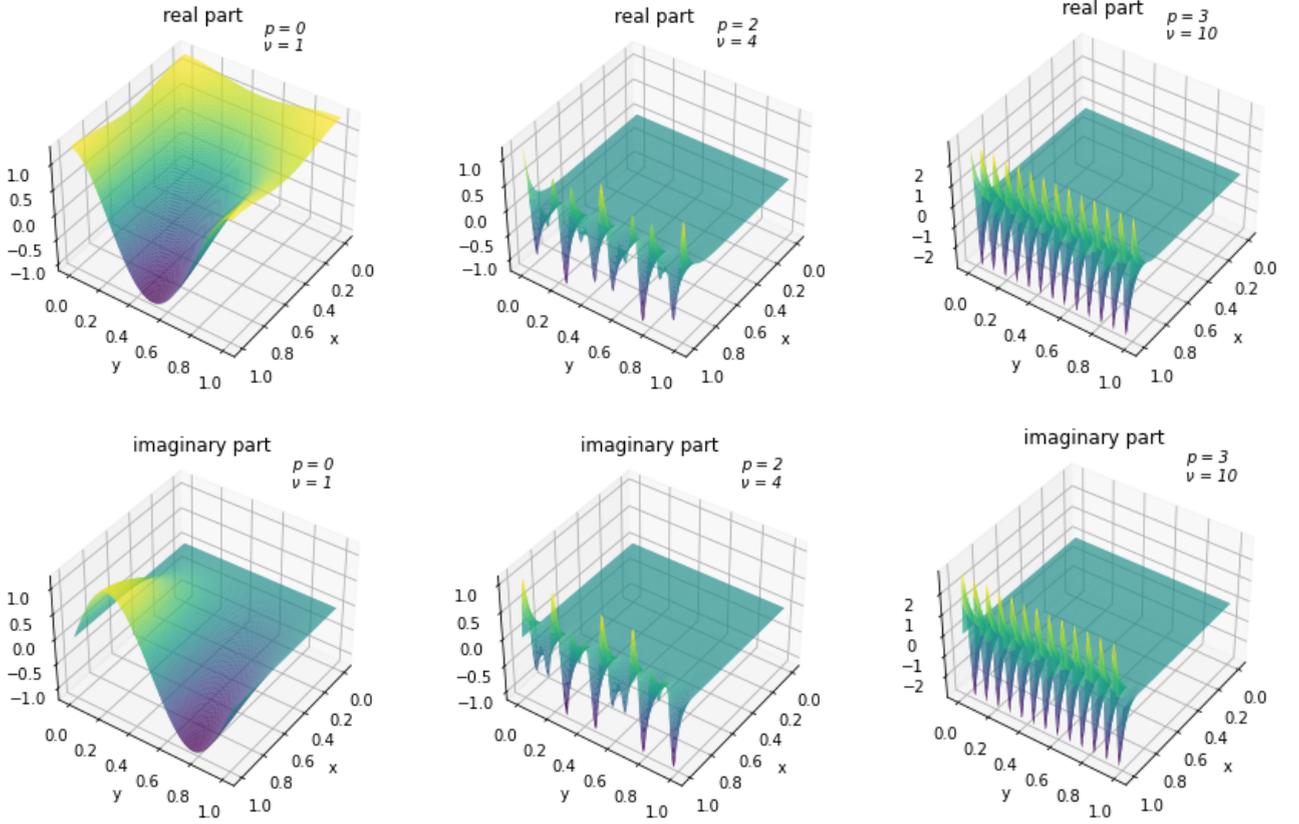


Fig. 1: Separate plots of the real and imaginary parts of three selected zero modes (19).

2.2. Raising and lowering operators

Now that the zero modes are determined, the higher modes are the next topic of interest. We found that there are ν zero modes for $A^\dagger A$ given by (19). Since we also know that the operators AA^\dagger and $A^\dagger A$ are related via a difference of $2B$ (11), every zero mode of $A^\dagger A$ implies one mode of AA^\dagger with the eigenvalue $2B$, of which are thus ν in total. But since AA^\dagger and $A^\dagger A$ have the same non-zero eigenvalues, this also implies ν modes for $A^\dagger A$ with the eigenvalue $2B$. So there are 2ν modes with eigenvalue $2B$ in total. This argument can be repeated indefinitely to eigenvalues $k2B$ with $k \in \mathbb{N}$ to each of which there correspond 2ν modes. The situation is depicted in figure 2.

We can use the relation (11) together with the eigenvalue equations of φ and χ (10) to find a relation

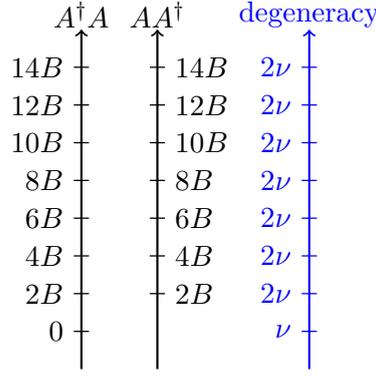


Fig. 2: Depiction of the eigenvalues of $A^\dagger A$ and AA^\dagger as well the amount of corresponding eigenmodes.

between φ and χ . We find that for $n \geq 1$

$$\begin{aligned}
 AA^\dagger \chi_{n,p} &= \lambda_n^2 \chi_{n,p} \\
 \iff (A^\dagger A + 2B) \chi_{n,p} &= \lambda_n^2 \chi_{n,p} \\
 \iff A^\dagger A \chi_{n,p} &= (\lambda_n^2 - 2B) \chi_{n,p} \\
 \iff A^\dagger A \chi_{n,p} &= \lambda_{n-1}^2 \chi_{n,p} .
 \end{aligned}$$

But this is just the eigenvalue equation of $\varphi_{n-1,p}$. This means

$$\varphi_{n-1,p} = \chi_{n,p} . \quad (20)$$

Using this relation we can further study the eigenvalue equations

$$\begin{aligned}
 AA^\dagger \chi_{n,p} &= \lambda_n^2 \chi_{n,p} \\
 \iff A^\dagger (AA^\dagger \chi_{n,p}) &= A^\dagger (\lambda_n^2 \chi_{n,p}) \\
 \iff A^\dagger A (A^\dagger \chi_{n,p}) &= \lambda_n^2 (A^\dagger \chi_{n,p}) \\
 \iff A^\dagger A \left(\frac{A^\dagger}{C_1(n)} \chi_{n,p} \right) &= \lambda_n^2 \left(\frac{A^\dagger}{C_1(n)} \chi_{n,p} \right) ,
 \end{aligned}$$

which is just the eigenvalue equation of $A^\dagger A$, as in (10). From this we find

$$\begin{aligned}
 \frac{A^\dagger}{C_1(n)} \chi_{n,p} &= \varphi_{n,p} \\
 \iff \frac{A^\dagger}{C_1(n)} \varphi_{n-1,p} &= \varphi_{n,p}
 \end{aligned}$$

and analogously we obtain

$$\frac{A}{C_2(n)} \varphi_{n,p} = \varphi_{n-1,p} .$$

So we can interpret A and A^\dagger as ladder operators. We introduced C_1 and C_2 so we have some freedom to ensure that the ladder operators can keep the normalization. So we have

$$A^\dagger \varphi_{n-1,p} = C_1(n) \varphi_{n,p} \quad \text{and} \quad A \varphi_{n,p} = C_2(n) \varphi_{n-1,p} . \quad (21)$$

Any other eigenmode can be obtained by using the ladder operators from equation (21). For convenience from now on we only write α_p instead of $\alpha_p + kBL$. From this notation the complete solution

can always be obtained by $\alpha_p \mapsto \alpha_p + kBL$ and summing over k . So, the first higher mode can be computed explicitly

$$\begin{aligned}\varphi_{1,p} &= \frac{1}{C_1(1)} A^\dagger \varphi_{0,p} \\ &= \frac{1}{C_1(1)} (iD_1 + D_2) \varphi_{0,p} \\ &= \frac{1}{C_1(1)} (i\partial_x + A_x + \partial_y - iA_y) \varphi_{0,p} \\ &= \frac{1}{C_1(1)} (i\partial_x - By + \partial_y) \varphi_{0,p} .\end{aligned}$$

With $\varphi_{0,p}$ explicitly inserted as in (19), we find

$$\begin{aligned}\varphi_{1,p} &= \frac{1}{C_1(1)} \sqrt[4]{\frac{B}{\pi L^2}} (i\partial_x - By + \partial_y) e^{i\alpha_p x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B})^2} \\ &= \frac{1}{C_1(1)} \sqrt[4]{\frac{B}{\pi L^2}} \left[-\alpha_p - By - B\left(y + \frac{\alpha_p}{B}\right) \right] e^{i\alpha_p x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B})^2} \\ &= -\frac{2B}{C_1(1)} \left(y + \frac{\alpha_p}{B}\right) \varphi_{0,p} .\end{aligned}$$

Now again, we can use $C_1(1)$ to normalize $\varphi_{1,p}$. Explicit computation and normalization of further eigenmodes leads to

$$C_1(1) = \sqrt{2B}, \quad C_1(2) = \sqrt{4B}, \quad C_1(3) = \sqrt{6B}, \quad C_1(4) = \sqrt{8B}, \quad \dots$$

which leads to the idea of the ansatz $C_1(n) = \sqrt{2nB} = \lambda_n$. With this we can write down an ansatz for any n th eigenmode by application of n raising operators

$$\begin{aligned}\varphi_{n,p} &= \frac{1}{\prod_{k=1}^n C_1(k)} (A^\dagger)^n \varphi_{0,p} \\ &= \frac{1}{\sqrt{n!}} \left(\frac{A^\dagger}{\sqrt{2B}} \right)^n \varphi_{0,p} .\end{aligned}$$

Here we can study the effect of n raising operators on the zero mode

$$\begin{aligned}(A^\dagger)^n \varphi_{0,p} &= (i\partial_x - By + \partial_y)^n \varphi_{0,p} \\ &= (-\alpha_p - By + \partial_y)^n \varphi_{0,p} \\ &= (-1)^n \sqrt{B}^n \left(\frac{\alpha_p}{\sqrt{B}} + \sqrt{B}y - \frac{\partial_y}{\sqrt{B}} \right)^n \varphi_{0,p} ,\end{aligned}$$

where we obtain via substitution $y' \equiv \frac{\alpha_p}{\sqrt{B}} + \sqrt{B}y$

$$\begin{aligned}(A^\dagger)^n \varphi_{0,p} &= (-1)^n \sqrt{B}^n (y' - \partial_{y'})^n \sqrt[4]{\frac{B}{\pi L^2}} e^{i\alpha_p x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B})^2} \\ &= \sqrt[4]{\frac{B}{\pi L^2}} e^{i\alpha_p x} (-1)^n \sqrt{B}^n (y' - \partial_{y'})^n e^{-\frac{y'^2}{2}} \\ &= \sqrt[4]{\frac{B}{\pi L^2}} e^{i\alpha_p x} (-1)^n \sqrt{B}^n e^{-\frac{y'^2}{2}} e^{\frac{y'^2}{2}} (y' - \partial_{y'})^n e^{-\frac{y'^2}{2}} .\end{aligned}$$

Here we can identify the Hermite polynomials $H_n(y')$ as they are given in (47) and also the zero modes $\varphi_{0,p}$ as they are given in (19)

$$\begin{aligned} &= (-1)^n \sqrt{B}^n H_n(y') \underbrace{\sqrt{\frac{B}{\pi L^2}} e^{i\alpha_p x} e^{-\frac{y'^2}{2}}}_{=\varphi_{0,p}} \\ &= (-1)^n \sqrt{B}^n H_n\left(\sqrt{B}y + \frac{\alpha_p}{\sqrt{B}}\right) \varphi_{0,p} \end{aligned}$$

which finally leads to the higher modes when remembering that $f(\alpha_p) \mapsto \sum_{k \in \mathbb{Z}} f(\alpha_p + kBL)$. For clear notation we introduce $\varphi_{0,p,k}$ such that $\varphi_{0,p} = \sum_{k \in \mathbb{Z}} \varphi_{0,p,k}$, which can directly be seen in (19). Thus, we get

Eigenmodes of the operator $A^\dagger A$ (9)

$$\varphi_{n,p} = \frac{1}{\sqrt{n!}} (-1)^n \frac{1}{\sqrt{2}^n} \sum_{k \in \mathbb{Z}} H_n\left(\sqrt{B}y + \frac{\alpha_p + kBL}{\sqrt{B}}\right) \varphi_{0,p,k} . \quad (22)$$

To check the orthonormality of our ansatz we compute the scalar product of any two eigenmodes. For this we use the orthogonality of the Hermite polynomials with respect to a weight function (50)

$$\begin{aligned} \langle H_n(y') \varphi_{0,p} | H_m(y') \varphi_{0,p} \rangle &= \sqrt{\frac{B}{\pi}} \int_{\mathbb{R}} H_n(y') H_m(y') e^{-B(y + \frac{\alpha_p}{B})^2} dy' \\ &= \sqrt{\frac{B}{\pi}} \int_{\mathbb{R}} H_n(y') H_m(y') e^{-y'^2} \frac{dy'}{\sqrt{B}} \\ &= \frac{1}{\sqrt{\pi}} \sqrt{\pi} 2^n n! \delta_{nm} \end{aligned} \quad (23)$$

which leads to

$$\begin{aligned} \langle \varphi_{n,p} | \varphi_{m,p} \rangle &= \frac{1}{n!} \frac{1}{2^n} \langle H_n(y') \varphi_{0,p} | H_m(y') \varphi_{0,p} \rangle \\ &= \delta_{nm} . \end{aligned}$$

This verifies the normalization.

These eigenmodes can also be represented in terms of Hermite functions, which is just an alternative notation. For this we use their form (22), the zero modes (19), $\alpha_p = \frac{2\pi p}{L}$, $B = \frac{\nu 2\pi}{L^2}$ and $\Phi = BL^2$ to obtain

Eigenmodes of the operator $A^\dagger A$ (9) represented by Hermite functions

$$\iff \varphi_{n,p} = \frac{(-1)^n}{\sqrt{2^n n!}} \sqrt{\frac{B}{\pi L^2}} \sum_{k \in \mathbb{Z}} \hat{H}_n\left(\sqrt{\Phi} \left(\frac{y}{L} + \frac{p + k\nu}{\nu}\right)\right) e^{2\pi i(p+k\nu)\frac{x}{L}} . \quad (24)$$

An explicit verification of the normalization of this alternative form can be found in appendix A.3. Before we go on to construct the eigenmodes of the Dirac operator, we want to study the zero modes a bit further. For later discretization attempts a study of the zeroes of the eigenmodes might be useful. Thus, the next chapter will be dedicated to the determination of the zeroes of the zero modes.

2.3. Zeroes of the zero modes

An explicit calculation of the zeroes is possible. This can be achieved by the identification of the so called *Jacobi theta function*, for which the zeroes are well known. A more detailed account on this function can be found in appendix A.4. To achieve an identification, consider the following rearrangement of the zero modes (19)

$$\varphi_{0,p}(x, y) = \sqrt[4]{\frac{B}{\pi L^2}} e^{i\alpha_p x - \frac{B}{2} y^2 - \frac{\alpha_p^2}{2B} - y\alpha_p} \sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(iBLx - BLy + \alpha_p L)} .$$

With this notation we can identify the Jacobi theta function as given in [12]

$$\vartheta(z, \tau) := \sum_{k \in \mathbb{Z}} e^{\pi i k^2 \tau + 2\pi i k z}$$

for $z \in \mathbb{C}$ and $\Im \tau > 0$. This leads to an representation of the zero modes with the theta function

$$\varphi_{0,p}(x, y) = \sqrt[4]{\frac{B}{\pi L^2}} e^{i\alpha_p x - \frac{B}{2} y^2 - \frac{\alpha_p^2}{2B} - y\alpha_p} \vartheta\left(i \frac{BLy - \alpha_p L}{2\pi} + \frac{BLx}{2\pi}, i \frac{BL^2}{2\pi}\right) .$$

This means, that the zeroes of the zero modes are given by the zeroes of the Jacobi theta function. As mentioned in (57), the zeroes of $\vartheta(z, \tau)$ are given by

$$z_{mn} = \left(m + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right)\tau, \quad m, n \in \mathbb{Z} .$$

This means for the above theta function the zeroes are given by the solutions of

$$i \frac{BLy - \alpha_p L}{2\pi} + \frac{BLx}{2\pi} = \left(m + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right) i \frac{BL^2}{2\pi} .$$

By comparison of the real and imaginary parts we find separate constraints for x and y when remembering that $B = \frac{\nu 2\pi}{L^2}$ and $\alpha_p = \frac{2\pi}{L} p$

$$y_n = \left(n + \frac{p}{\nu} + \frac{1}{2}\right)L$$

and

$$x_m = \left(m + \frac{1}{2}\right) \frac{L}{\nu} .$$

But since we are constrained to a square we obtain a finite amount of zeroes depending on p and ν . For x_m we find exactly ν zeroes at

$$x_m = \left(m + \frac{1}{2}\right) \frac{L}{\nu}, \quad m \in [0, \nu - 1] .$$

For y_n we find

$$\begin{aligned} 0 &\leq \left(n + \frac{p}{\nu} + \frac{1}{2}\right)L \leq L \\ \iff -\frac{1}{2} - \frac{p}{\nu} &\leq n \leq \frac{1}{2} - \frac{p}{\nu} . \end{aligned}$$

The maximum value for $\frac{p}{\nu}$ is 1. We have three cases. For those we get the zeroes

$$n \in \begin{cases} \{-1\} & , \frac{p}{\nu} > \frac{1}{2} \\ \{-1, 0\} & , \frac{p}{\nu} = \frac{1}{2} \\ \{0\} & , \frac{p}{\nu} < \frac{1}{2} \end{cases}$$

which means for y_n we have the zeroes

$$y_0 = \left(\frac{p}{\nu} - \frac{1}{2}\right)L, \quad \frac{p}{\nu} \geq \frac{1}{2}$$

$$y_1 = \left(\frac{p}{\nu} + \frac{1}{2}\right)L, \quad \frac{p}{\nu} \leq \frac{1}{2}.$$

This means that in total we have ν zeroes for $\frac{p}{\nu} \neq \frac{1}{2}$, which are located on the inside. Also, we have 2ν zeroes for $\frac{p}{\nu} = \frac{1}{2}$, which are all located on the boundary in y -direction.

Zeroes of the zero modes (19)

$$x_m = \left(m + \frac{1}{2}\right)\frac{L}{\nu}, \quad m \in [0, \nu - 1]$$

$$y_0 = \left(\frac{p}{\nu} - \frac{1}{2}\right)L, \quad \frac{p}{\nu} \geq \frac{1}{2}$$

$$y_1 = \left(\frac{p}{\nu} + \frac{1}{2}\right)L, \quad \frac{p}{\nu} \leq \frac{1}{2}.$$

A check of this result by application of the *residue theorem* can be found in appendix A.5. This now concludes the study of the eigenmodes $\varphi_{n,p}$. Out of those the eigenmodes of the original Dirac operator can be constructed.

2.4. Eigenfunctions of the Dirac operator

Now we want to finally determine the eigenmodes of the original Dirac operator (7) out of the determined eigenmodes (22) of the squared Dirac operator (8). As we have already seen before in equation (12), the eigenfunctions of $-\mathcal{D}^2$ factorize into t - and x -dependent parts. The corresponding eigenvalues are thus $\mu_n^2 = \omega^2 + \lambda_n^2$. The orthonormal eigenfunctions of the Dirac operator $i\mathcal{D}$ can be derived directly from the ones of the squared operator $(i\mathcal{D})^2$ to be

Eigenmodes of the Dirac operator (7)

$$\varphi_{\omega,n,p} = \frac{1}{\sqrt{2\beta}} e^{i\omega x^0} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p} \\ \lambda\chi_{n,p} \end{pmatrix}$$

$$\chi_{\omega,n,p} = \frac{1}{\sqrt{2\beta}} e^{i\omega x^0} \frac{1}{\sqrt{\mu_n(\mu_n + \omega)}} \begin{pmatrix} \lambda\varphi_{n,p} \\ (\mu_n + \omega)\chi_{n,p} \end{pmatrix}$$

where the eigenvalues come in pairs $\mu_n = \pm\sqrt{\omega^2 + \lambda_n^2}$. These two modes are proportional to each

other

$$\begin{aligned}
 \varphi_{\omega,n,p} &= \frac{1}{\sqrt{2\beta}} e^{i\omega x^0} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p} \\ \lambda\chi_{n,p} \end{pmatrix} \cdot \frac{\mu_n + \omega}{\mu_n + \omega} \\
 &= \frac{1}{\sqrt{2\beta}} e^{i\omega x^0} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} \lambda_n^2 \varphi_{n,p} \\ \lambda_n(\mu_n + \omega)\chi_{n,p} \end{pmatrix} \cdot \frac{1}{\mu_n + \omega} \\
 &= \frac{\lambda_n}{\mu_n + \omega} \chi_{\omega,n,p}
 \end{aligned}$$

and thus denote the same solution. This means, it is enough to consider only $\varphi_{\omega,n,p}$, since they are just the same eigenfunction. It can be checked that $\varphi_{\omega,n,p}$ is indeed an eigenfunction

$$\begin{aligned}
 i\mathcal{D}\varphi_{\omega,n,p} &= \begin{pmatrix} i\partial_0 & A^\dagger \\ A & -i\partial_0 \end{pmatrix} \frac{1}{\sqrt{2\beta}} e^{i\omega x^0} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p} \\ \lambda_n\chi_{n,p} \end{pmatrix} \\
 &= e^{i\omega x^0} \frac{1}{\sqrt{2\beta}} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} -\omega(\mu_n - \omega)\varphi_{n,p} + \lambda_n A^\dagger \chi_{n,p} \\ (\mu_n - \omega)A\varphi_{n,p} + \lambda_n \omega \chi_{n,p} \end{pmatrix}
 \end{aligned}$$

where we have to use the relation between $\varphi_{n,p}$ and $\chi_{n,p}$ as given in (20)

$$\begin{aligned}
 i\mathcal{D}\varphi_{\omega,n,p} &= e^{i\omega x^0} \frac{1}{\sqrt{2\beta}} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} -\omega(\mu_n - \omega)\varphi_{n,p} + \lambda_n^2 \varphi_{n,p} \\ (\mu_n - \omega)\lambda_n \chi_{n,p} + \lambda_n \omega \chi_{n,p} \end{pmatrix} \\
 &= e^{i\omega x^0} \frac{1}{\sqrt{2\beta}} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \begin{pmatrix} (\mu_n - \omega)[-\omega + \mu_n + \omega]\varphi_{n,p} \\ \mu_n \lambda \chi_{n,p} \end{pmatrix} \\
 &= \mu_n \varphi_{\omega,n,p} .
 \end{aligned}$$

A verification of the normalization of these eigenmodes can be found in appendix A.3. In the next chapter we will need the spectral decomposition of the Dirac operator. Here, the sum over μ means the sum over the sign pairs of the eigenvalues μ_n

$$\langle x | i\mathcal{D} | y \rangle := \sum_{\omega,n,p,\mu} \mu_n \varphi_{\omega,n,p}(x) \varphi_{\omega,n,p}^\dagger(y) . \quad (25)$$

This is why we also note the following result

$$\begin{aligned}
 \varphi_{\omega,n,p}(x) \varphi_{\omega,n,p}^\dagger(y) &= \frac{e^{i\omega(x_0 - y_0)}}{2\beta} \frac{1}{\mu_n(\mu_n - \omega)} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p}(\vec{x}) \\ \lambda_n \chi_{n,p}(\vec{x}) \end{pmatrix} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\
 &= \frac{e^{i\omega(x_0 - y_0)}}{2\beta} \frac{1}{\mu_n} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p}(\vec{x})\varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x})\chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x})\varphi_{n,p}^\dagger(\vec{y}) & (\mu_n + \omega)\chi_{n,p}(\vec{x})\chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} . \quad (26)
 \end{aligned}$$

At this point the eigenmodes and -values of the Dirac operator have been determined, checked and studied quite extensively. The final section of this thesis will now present an attempt to achieve a discretization of this operator.

3. Discretization of the Dirac operator

This chapter will present an attempt of finding a discretization of the Dirac operator (7). Currently, all determined objects depend on the continuous variables of space and time. To be able to apply numerical methods we need to only depend on discrete coordinates, which is why we want to move on a lattice. For this we will use its spectral decomposition (25). The Dirac operator in question is of $2+1$ dimensions and section 2 has revealed, that the operator is periodic in time and one space direction. The second space direction is more complicated. We will first study the discretization of the time direction in chapter 3.1, for which we use the concept of the *SLAC-derivative*. After that, we simplify the ensuing term for the operator in chapter 3.2, while also noting a few alternative representations in chapter 3.3. We hope to find a discretization of the non-periodic space direction by studying how the Gaussian quadrature can be applied to it. Chapter 3.4 presents a verification, that the eigenvalue equation of the Dirac operator still holds on a fitting quadrature grid. Finally, the last chapter 3.5 presents an attempt of explicitly writing down a fitting grid, while trying to analyze the ensuing problems.

3.1. Spectral resolution

We wish to discretize the time direction, which is periodic. For this we use the concept of the *SLAC-derivative*, as introduced in [13] and [14]. For this we consider the operator $i\mathcal{D}$ in position space. Thus, the relation of interest is (26), from which the important factor is $e^{i\omega(x_0-y_0)}$, where we define the time difference as $\xi \equiv x_0 - y_0$. We study the sum of $e^{i\omega(x_0-y_0)}$ over the *Matsubara frequencies* $\omega_m = 2\pi \frac{m+\frac{1}{2}}{\beta}$ with $m \in \mathbb{Z}$ symmetric to $\omega = 0$. The interval of interest for an even number of frequencies N_t is then given by $m \in [-\frac{N_t}{2}, \frac{N_t}{2} - 1]$. To obtain a SLAC-derivative we cut off the sum symmetric to the origin

$$\begin{aligned} \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} e^{i\omega_m \xi} &= \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} e^{i2\pi \frac{m+\frac{1}{2}}{\beta} \xi} \\ &= e^{i\pi \frac{\xi}{\beta}} (e^{i2\pi \frac{1}{\beta} \xi})^{-\frac{N_t}{2}} \sum_{m=0}^{N_t-1} (e^{i2\pi \frac{\xi}{\beta}})^m, \end{aligned}$$

where the ensuing geometric series leads to

$$\begin{aligned} \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} e^{i\omega_m \xi} &= e^{i\pi \frac{\xi}{\beta}} e^{-i\pi \frac{N_t}{\beta} \xi} \frac{1 - (e^{i2\pi \frac{\xi}{\beta}})^{N_t}}{1 - e^{i2\pi \frac{\xi}{\beta}}} \\ &= \frac{\sin(\pi \frac{N_t}{\beta} \xi)}{\sin(\pi \frac{\xi}{\beta})}. \end{aligned} \quad (27)$$

Differentiating this equation with respect to ξ yields

$$\begin{aligned} i \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} \omega_m e^{i\omega_m \xi} &= \frac{\pi N_t}{\beta} \frac{\cos(\pi N_t \frac{\xi}{\beta})}{\sin(\pi \frac{\xi}{\beta})} - \frac{\pi}{\beta} \frac{\sin(\pi N_t \frac{\xi}{\beta}) \cos(\pi \frac{\xi}{\beta})}{\sin^2(\pi \frac{\xi}{\beta})} \\ &= \frac{\pi}{\beta} \left(N_t \frac{\cos(\pi N_t \frac{\xi}{\beta})}{\sin(\pi \frac{\xi}{\beta})} - \frac{\sin(\pi N_t \frac{\xi}{\beta}) \cos(\pi \frac{\xi}{\beta})}{\sin^2(\pi \frac{\xi}{\beta})} \right). \end{aligned} \quad (28)$$

Now we go on to discretize the interval $[0, \beta]$ by N_t sites, which leads to

$$\xi \mapsto \xi_{ss'} = \frac{\beta}{N_t}(s - s') \quad \text{and} \quad t_{ss'} \equiv \frac{\pi}{\beta}\xi_{ss'} = \frac{\pi}{N_t}(s - s').$$

with $s, s' \in \{0, \dots, N_t\}$. This way we find for the spectral sum (27)

$$\begin{aligned} \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} e^{i\omega_m \xi_{ss'}} &= \frac{\sin(\pi N_t \frac{\xi_{ss'}}{\beta})}{\sin(\pi \frac{\xi_{ss'}}{\beta})} \\ &= \frac{\sin[\pi(s - s')]}{\sin[\frac{\pi}{N_t}(s - s')]} \end{aligned}$$

Here the numerator becomes zero for any s and s' , but the denominator does so only for $s - s' = N_t \mathbb{Z}$. To find the limit when both become zero we can use *L'Hôpital's rule*

$$\lim_{x \rightarrow 0} \frac{\sin[\pi x]}{\sin[\frac{\pi}{N_t} x]} = N_t \lim_{x \rightarrow 0} \frac{\cos[\pi x]}{\cos[\frac{\pi}{N_t} x]} = N_t$$

which leads to

$$\sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} e^{i\omega_m \xi_{ss'}} = N_t \delta_{ss'} \quad (29)$$

where $\delta_{ss'}$ is the Kronecker symbol on \mathbb{Z}_{N_t} . If we now analyze the derivative of the spectral sum (28) we can define a matrix, which is the so called SLAC-derivative

$$\begin{aligned} i \sum_{m=-\frac{N_t}{2}}^{\frac{N_t}{2}-1} \omega_m e^{i\omega_m \xi_{ss'}} &= \frac{\pi}{\beta} \left(N_t \frac{\cos[\pi(s - s')]}{\sin[\frac{\pi}{N_t}(s - s')]} - \frac{\sin[\pi(s - s')] \cos[\frac{\pi}{N_t}(s - s')]}{\sin^2[\frac{\pi}{N_t}(s - s')]} \right) \\ &= \frac{N_t \pi}{\beta} \frac{1}{\sin t_{ss'}} \left\{ \underbrace{(-1)^{s-s'}}_{=1 \text{ for } s=s'} - \delta_{ss'} \underbrace{\cos\left[\frac{\pi}{N_t}(s - s')\right]}_{=1 \text{ for } s=s'} \right\} \\ &= \frac{N_t \pi}{\beta} \frac{(-1)^{s-s'}}{\sin t_{ss'}} (1 - \delta_{ss'}) := N_t \partial_{\text{slac}, ss'}. \end{aligned} \quad (30)$$

Now we can apply this to the spectral decomposition (25) of the Dirac operator with (26)

$$\langle x | i\mathcal{D} | y \rangle = \sum_m \frac{e^{i\omega_m(x_0 - y_0)}}{2\beta} \sum_{n,p,\mu} \begin{pmatrix} (\mu_n - \omega_m) \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & (\mu_n + \omega_m) \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix}$$

to effectively discretize the time direction. Since the eigenvalues μ_n come in pairs with opposite sign and n runs through the natural numbers \mathbb{N} we can simplify the sum to

Spectral decomposition of the Dirac operator (7) with discretized time direction

$$\langle x | i\mathcal{D} | y \rangle = \sum_m \frac{e^{i\omega_m(x_0 - y_0)}}{\beta} \sum_{n,p} \begin{pmatrix} -\omega_m \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \omega_m \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix}. \quad (31)$$

We can check this result by acting with $i\mathcal{D}$ on it, where the index x denotes, that the derivatives are in respect to x

$$\begin{aligned} i\mathcal{D}_x \langle x | i\mathcal{D} | y \rangle &= \begin{pmatrix} i\partial_{x_0} & A_x^\dagger \\ A_x & -i\partial_{x_0} \end{pmatrix} \sum_m \frac{e^{i\omega_m(x_0-y_0)}}{\beta} \sum_{n,p} \begin{pmatrix} -\omega_m \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \omega_m \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\ &= \sum_{m,n,p} \frac{e^{i\omega_m(x_0-y_0)}}{\beta} \underbrace{\begin{pmatrix} -\omega_m & A_x^\dagger \\ A_x & \omega_m \end{pmatrix} \begin{pmatrix} -\omega_m \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \omega_m \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix}}_{\equiv M}. \end{aligned}$$

The first and second matrix elements here are

$$\begin{aligned} M_{11} &= \omega_m^2 \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) + \lambda_n \underbrace{[A_x^\dagger \chi_{n,p}(\vec{x})]}_{=\lambda_n \varphi_{n,p}(\vec{x})} \varphi_{n,p}^\dagger(\vec{y}) = (\omega_m^2 + \lambda_n^2) \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) \\ M_{21} &= -\omega_m \underbrace{[A_x \varphi_{n,p}(\vec{x})]}_{=\lambda_n \chi_{n,p}(\vec{x})} \varphi_{n,p}^\dagger(\vec{y}) + \omega_m \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) = 0. \end{aligned}$$

The other two matrix elements can be calculated analogously to give

$$\begin{aligned} i\mathcal{D}_x \langle x | i\mathcal{D} | y \rangle &= \sum_{m,n,p} \frac{e^{i\omega_m(x_0-y_0)}}{\beta} (\omega_m^2 + \lambda_n^2) \begin{pmatrix} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & 0 \\ 0 & \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\ &= \langle x | (i\mathcal{D})^2 | y \rangle. \end{aligned}$$

which indeed gives the spectral decomposition of the squared operator. With the SLAC-derivative we have found above (30) we can get rid of one sum in the spectral decomposition (31) when going on a lattice. The operator is now discretized in the time direction. The time integral when evaluating scalar products turns into a sum over the grid points which are separated by $\frac{\beta}{N_t}$. We also multiply by the factor $\frac{\beta}{N_t}$ so they are separated by 1

$$\begin{aligned} \langle \vec{x}, s | i\mathcal{D} | \vec{y}, s' \rangle &= \frac{\beta}{N_t} \sum_m \frac{e^{i\omega_m \xi_{ss'}}}{\beta} \sum_{n,p} \begin{pmatrix} -\omega_m \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & \omega_m \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\ &= \sum_m \frac{1}{N_t} \omega_m e^{i\omega_m \xi_{ss'}} \sum_{n,p} \begin{pmatrix} -\varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & 0 \\ 0 & \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\ &\quad + \sum_m \frac{1}{N_t} e^{i\omega_m \xi_{ss'}} \sum_{n,p} \lambda_n \begin{pmatrix} 0 & \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & 0 \end{pmatrix} \end{aligned}$$

which leads to

Spectral decomposition of the Dirac operator (7) after application of the SLAC-derivative

$$\begin{aligned} \langle \vec{x}, s | i\mathcal{D} | \vec{y}, s' \rangle &= \frac{\pi}{i\beta} \frac{(-1)^{s-s'}}{\sin t_{ss'}} (1 - \delta_{ss'}) \sum_{n,p} \begin{pmatrix} -\varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & 0 \\ 0 & \chi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \end{pmatrix} \\ &\quad + \delta_{ss'} \sum_{n,p} \lambda_n \begin{pmatrix} 0 & \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) \\ \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) & 0 \end{pmatrix}. \end{aligned} \quad (32)$$

3.2. Simplifying the spectral sum

We wish to further simplify the spectral sum (32), since the triple sum over n and two times k inside of $\varphi_{n,p}$ and $\chi_{n,p}$ can lead to numerical problems. We ignore the sum over p for now, since its size depends on the strength of the magnetic field. For the simplification we can use the *Christoffel-Darboux formula* for the Hermite polynomials

$$\sum_{n=0}^N \frac{H_n(x)H_n(y)}{2^n n!} = \frac{1}{2^{N+1}N!} \frac{H_N(y)H_{N+1}(x) - H_N(x)H_{N+1}(y)}{x-y}, \quad (33)$$

as can be found in [11]. Using the recursion relation for Hermite polynomials (49), we can use L'Hôpital's rule to find a symmetric form of the Christoffel-Darboux formula

$$\begin{aligned} \sum_{n=0}^N \frac{H_n(x)H_n(x)}{2^n n!} &= \frac{1}{2^{N+1}N!} \lim_{y \rightarrow x} \frac{H_N(y)H_{N+1}(x) - H_N(x)H_{N+1}(y)}{x-y} \\ &= \frac{1}{2^{N+1}N!} [H_N(x)H'_{N+1}(x) - H'_N(x)H_{N+1}(x)] \\ &= \frac{1}{2^N N!} [(N+1)H_N^2 - NH_{N-1}H_{N+1}] \end{aligned}$$

which can also be written as

$$\sum_{n=0}^{N-1} \frac{H_n(x)H_n(x)}{2^n n!} = \frac{1}{2^N(N-1)!} [H_N^2 - H_{N-1}H_{N+1}].$$

We begin by analyzing the first matrix element of the spectral sum (32). For this we use the explicit form of the modes $\varphi_{n,p}$ (22), the shifted summation index $b = k' - k$ and $x_{p,k} = \sqrt{\Phi} \left(\frac{x_2}{L} + \frac{p+k\nu}{\nu} \right)$

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) &= \sqrt{\frac{B}{\pi L^2}} \sum_{n,p} \sum_{k,b} \frac{1}{2^n n!} H_n(x_{p,k}) H_n(y_{p,k+b}) e^{i(\alpha_p + kBL)x_1} e^{-\frac{B}{2}(x_2 + \frac{\alpha_p}{B} + kL)^2} \\ &\quad \cdot e^{-i(\alpha_p + (k+b)BL)y_1} e^{-\frac{B}{2}(y_2 + \frac{\alpha_p}{B} + (k+b)L)^2} \\ &= \sqrt{\frac{B}{\pi L^2}} \sum_{n,p} \sum_{k,b} \frac{1}{2^n n!} H_n(x_{p,k}) H_n(y_{p,k+b}) e^{i\frac{2\pi}{L}(p+k\nu)(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{x_{p,k}^2}{2}} e^{-\frac{y_{p,k+b}^2}{2}}. \end{aligned}$$

We can get rid of the summation over p by using the identity

$$\sum_{k \in \mathbb{Z}} \sum_{p=1}^{\nu} f(p+k\nu) = \sum_{a \in \mathbb{Z}} f(a)$$

which gives

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) &= \sqrt{\frac{B}{\pi L^2}} \sum_{a,b} \sum_{n=0}^N \frac{1}{2^n n!} H_n \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_n \left[\sqrt{B} \left(y_2 + \frac{aL}{\nu} + bL \right) \right] \\ &\quad \cdot e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} \right)^2} e^{-\frac{B}{2} \left(y_2 + \frac{aL}{\nu} + bL \right)^2} \end{aligned}$$

where we can now apply Christoffel-Darboux (33)

$$\begin{aligned}
 \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= \sqrt{\frac{1}{\pi L^2}} \sum_{a,b} \frac{1}{2^{N+1} N!} \frac{1}{x_2 - y_2 - bL} \\
 &\cdot \left\{ H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_N \left[\sqrt{B} \left(y_2 + \frac{aL}{\nu} + bL \right) \right] \right. \\
 &\quad \left. - H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_{N+1} \left[\sqrt{B} \left(y_2 + \frac{aL}{\nu} + bL \right) \right] \right\} \\
 &\cdot e^{i \frac{2\pi}{L} a(x_1 - y_1)} e^{-i \frac{2\pi}{L} \nu b y_1} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} \right)^2} e^{-\frac{B}{2} \left(y_2 + \frac{aL}{\nu} + bL \right)^2} . \tag{34}
 \end{aligned}$$

Now we got rid of the sums over p and n . To check this result, the explicit calculations from appendix A.6 lead to

$$\int_{L^2} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{x}) \, d\vec{x} = \nu(N+1) , \tag{35}$$

which is just the number of summands and thus the expected result. We can simplify the spectral sum (34) marginally by defining the magnetic length $\ell_m = \frac{1}{\sqrt{B}}$ as a unit length. Thus, all lengths are given in multiples of this value

First matrix element of the spectral decomposition (31) after application of Christoffel-Darboux

$$\begin{aligned}
 \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= \sqrt{\frac{1}{\pi L^2}} \sum_{a,b} \frac{B}{2^{N+1} N!} \frac{1}{x_2 - y_2 - bL} \left[H_{N+1} \left(x_2 + \frac{aL}{\nu} \right) H_N \left(y_2 + \frac{aL}{\nu} + bL \right) \right. \\
 &\quad \left. - H_N \left(x_2 + \frac{aL}{\nu} \right) H_{N+1} \left(y_2 + \frac{aL}{\nu} + bL \right) \right] \\
 &\cdot e^{i \frac{2\pi}{L} a(x_1 - y_1)} e^{-i \frac{2\pi}{L} \nu b y_1} e^{-\frac{1}{2} \left(x_2 + \frac{aL}{\nu} \right)^2} e^{-\frac{1}{2} \left(y_2 + \frac{aL}{\nu} + bL \right)^2} . \tag{36}
 \end{aligned}$$

Now we go on to compute the other matrix elements of (32), where the sum over n now starts from 1

$$\begin{aligned}
 \sum_{n,p} \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= \sum_{n,p} \lambda_n \varphi_{n-1,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) \\
 &= -\sqrt{\frac{B^2}{\pi L^2}} \sum_{n,p} \sum_{k,b} \frac{1}{2^{n-1} (n-1)!} H_{n-1}(x_{p,k}) H_n(y_{p,k+b}) e^{i \frac{2\pi}{L} (p+k\nu)(x_1 - y_1)} e^{-i \frac{2\pi}{L} \nu b y_1} \\
 &\quad \cdot e^{-\frac{x_{p,k}^2}{2}} e^{-\frac{y_{p,k+b}^2}{2}} .
 \end{aligned}$$

Let us focus on the sum over the Hermite polynomials, so we find a way to use the Christoffel-Darboux

formula. We first use the recursion relation (49) again

$$\begin{aligned}
 \sum_{n=1}^N \frac{H_{n-1}(x_{p,k})H_n(y_{p,k+b})}{2^{n-1}(n-1)!} &= \sum_{n=1}^N \frac{1}{2^n n!} H'_n(x_{p,k})H_n(y_{p,k+b}) \\
 &= \frac{1}{\sqrt{B}} \partial_{x_2} \sum_{n=1}^N \frac{1}{2^n n!} H_n(x_{p,k})H_n(y_{p,k+b}) \\
 &= \frac{1}{\sqrt{B}} \partial_{x_2} \left[\sum_{n=0}^N \frac{1}{2^n n!} H_n(x_{p,k})H_n(y_{p,k+b}) - H_0(x_{p,k})H_0(y_{p,k+b}) \right]
 \end{aligned} \tag{37}$$

and are now able to apply Christoffel-Darboux (33)

$$\begin{aligned}
 \sum_{n=1}^N \frac{H_{n-1}(x_{p,k})H_n(y_{p,k+b})}{2^{n-1}(n-1)!} &= \frac{1}{\sqrt{B}} \partial_{x_2} \left[\frac{1}{2^{N+1}N!} \frac{H_N(y_{p,k+b})H_{N+1}(x_{p,k}) - H_N(x_{p,k})H_{N+1}(y_{p,k+b})}{x_{p,k} - y_{p,k+b}} \right. \\
 &\quad \left. - \underbrace{H'_0(x_{p,k})}_{=0} H_0(y_{p,k+b}) \right] \\
 &= \frac{1}{2^{N+1}N! \sqrt{B}} \partial_{x_2} \left[\frac{H_N(y_{p,k+b})H_{N+1}(x_{p,k}) - H_N(x_{p,k})H_{N+1}(y_{p,k+b})}{x_{p,k} - y_{p,k+b}} \right].
 \end{aligned}$$

So with that and again introducing $a = k + p\nu$ we find for the second matrix element

$$\begin{aligned}
 \sum_{n,p} \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) &= -\sqrt{\frac{B}{\pi L^2}} \frac{1}{2^{N+1}N!} \sum_{a,b} e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{B}{2}(x_2 + \frac{aL}{\nu})^2} e^{-\frac{B}{2}(y_2 + \frac{aL}{\nu} + bL)^2} \\
 &\quad \cdot \partial_{x_2} \left[\frac{H_N[\sqrt{B}(y_2 + \frac{aL}{\nu} + bL)]H_{N+1}[\sqrt{B}(x_2 + \frac{aL}{\nu})]}{\sqrt{B}(x_2 - y_2 - bL)} \right. \\
 &\quad \left. - \frac{H_N[\sqrt{B}(x_2 + \frac{aL}{\nu})]H_{N+1}[\sqrt{B}(y_2 + \frac{aL}{\nu} + bL)]}{\sqrt{B}(x_2 - y_2 - bL)} \right]
 \end{aligned}$$

and finally by also rescaling to units of ℓ_m , we arrive at the form

Second matrix element of the spectral decomposition (31) after application of Christoffel-Darboux

$$\begin{aligned}
 \sum_{n,p} \lambda_n \chi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) &= -\sqrt{\frac{1}{\pi L^2}} \frac{B^{\frac{3}{2}}}{2^{N+1}N!} \sum_{a,b} e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{1}{2}(x_2 + \frac{aL}{\nu})^2} e^{-\frac{1}{2}(y_2 + \frac{aL}{\nu} + bL)^2} \\
 &\quad \cdot \partial_{x_2} \left[\frac{H_N(y_2 + \frac{aL}{\nu} + bL)H_{N+1}(x_2 + \frac{aL}{\nu})}{x_2 - y_2 - bL} \right. \\
 &\quad \left. - \frac{H_N(x_2 + \frac{aL}{\nu})H_{N+1}(y_2 + \frac{aL}{\nu} + bL)}{x_2 - y_2 - bL} \right].
 \end{aligned} \tag{38}$$

In a similar fashion we compute the last matrix element

$$\begin{aligned}
 \sum_{n,p} \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) &= \sum_{n,p} \lambda_n \varphi_{n,p}(\vec{x}) \varphi_{n-1,p}^\dagger(\vec{y}) \\
 &= \sqrt{\frac{B}{\pi L^2}} \sum_{n,p} \sum_{k,b} \frac{-\sqrt{2nB}}{\sqrt{2^n n! 2^{n-1} (n-1)!}} H_n(x_{p,k})H_{n-1}(y_{p,k+b}) e^{i\frac{2\pi}{L}(p+k\nu)(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} \\
 &\quad \cdot e^{-\frac{x_{p,k}^2}{2}} e^{-\frac{y_{p,k+b}^2}{2}}.
 \end{aligned}$$

which has the same form as the the calculation before, only with the arguments in the Hermite polynomials swapped. Thus, the solution is the same, with only the derivative changing to be in respect to the other space coordinate. The relevant step for this is at (37). So, the solution is

Third matrix element of the spectral decomposition (31) after application of Christoffel-Darboux

$$\begin{aligned} \sum_{n,p} \lambda_n \varphi_{n,p}(\vec{x}) \chi_{n,p}^\dagger(\vec{y}) &= -\sqrt{\frac{1}{\pi L^2}} \frac{B^{\frac{3}{2}}}{2^{N+1} N!} \sum_{a,b} e^{i\frac{2\pi}{L} a(x_1-y_1)} e^{-i\frac{2\pi}{L} \nu b y_1} e^{-\frac{1}{2}\left(x_2+\frac{aL}{\nu}\right)^2} e^{-\frac{1}{2}\left(y_2+\frac{aL}{\nu}+bL\right)^2} \\ &\cdot \partial_{y_2} \left[\frac{H_N\left(y_2+\frac{aL}{\nu}+bL\right) H_{N+1}\left(x_2+\frac{aL}{\nu}\right)}{x_2-y_2-bL} \right. \\ &\quad \left. - \frac{H_N\left(x_2+\frac{aL}{\nu}\right) H_{N+1}\left(y_2+\frac{aL}{\nu}+bL\right)}{x_2-y_2-bL} \right]. \end{aligned} \quad (39)$$

So, altogether the fully simplified spectral decomposition (31) is given by the explicit matrix elements (36), (38) and (39). This expression is quite unwieldy. There do not seem to be any further obvious simplifications, but there still can be some benefit in considering an alternative form. Thus, the next chapter will shortly present a few different representations, which might have an advantage in further study.

3.3. Alternative representations of the first matrix element

The first matrix element of the Dirac operator (36) has been calculated in chapter 3.2 to be

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^\dagger(\vec{y}) &= C \sum_{a,b} \frac{1}{x_2-y_2-bL} \left[H_{N+1}\left(x_2+\frac{aL}{\nu}\right) H_N\left(y_2+\frac{aL}{\nu}+bL\right) \right. \\ &\quad \left. - H_N\left(x_2+\frac{aL}{\nu}\right) H_{N+1}\left(y_2+\frac{aL}{\nu}+bL\right) \right] \\ &\cdot e^{i\frac{2\pi}{L} a(x_1-y_1)} e^{-i\frac{2\pi}{L} \nu b y_1} e^{-\frac{1}{2}\left(x_2+\frac{aL}{\nu}\right)^2} e^{-\frac{1}{2}\left(y_2+\frac{aL}{\nu}+bL\right)^2}. \end{aligned} \quad (40)$$

where C summarizes the constants. For a sum as an argument inside of Hermite polynomials the following identity holds [15]

$$H_n(x+y) = \sum_{k=0}^n \binom{n}{k} x^k H_{n-k}(y). \quad (41)$$

With this we could rewrite the factor with the Hermite polynomials from (40)

$$\begin{aligned} &H_{N+1}\left(x_2+\frac{aL}{\nu}\right) H_N\left(y_2+\frac{aL}{\nu}+bL\right) - H_N\left(x_2+\frac{aL}{\nu}\right) H_{N+1}\left(y_2+\frac{aL}{\nu}+bL\right) \\ &= \sum_{k=0}^{N+1} \sum_{l=0}^N \binom{N+1}{k} \binom{N}{l} \left[\left(\frac{aL}{\nu}\right)^k H_{N+1-k}(x_2) \left(\frac{aL}{\nu}+bL\right)^l H_{N-l}(y_2) \right. \\ &\quad \left. - \left(\frac{aL}{\nu}\right)^l H_{N-l}(x_2) \left(\frac{aL}{\nu}+bL\right)^k H_{N+1-k}(y_2) \right] \end{aligned}$$

which gives overall a form with only the coordinates as arguments of the Hermite polynomials

First matrix element of the spectral decomposition (31) with the coordinates as arguments of the Hermite polynomials

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= C \sum_{a,b} \sum_{k=0}^{N+1} \sum_{l=0}^N \binom{N+1}{k} \binom{N}{l} e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{1}{2}\left(x_2+\frac{aL}{\nu}\right)^2} \\ &\quad e^{-\frac{1}{2}\left(y_2+\frac{aL}{\nu}+bL\right)^2} \frac{\left(\frac{aL}{\nu}\right)^k H_{N+1-k}(x_2) \left(\frac{aL}{\nu}+bL\right)^l H_{N-l}(y_2)}{x_2 - y_2 - bL} \\ &\quad - \frac{\left(\frac{aL}{\nu}\right)^l H_{N-l}(x_2) \left(\frac{aL}{\nu}+bL\right)^k H_{N+1-k}(y_2)}{x_2 - y_2 - bL}. \end{aligned}$$

Alternatively, a form with the same argument inside of all Hermite polynomials could be of interest. For this, one could isolate $\frac{aL}{\nu}$ inside the Hermite polynomials from (40) by again using (41) to obtain

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= C \sum_{a,b} \sum_{k=0}^{N+1} \sum_{l=0}^N \binom{N+1}{k} \binom{N}{l} e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{1}{2}\left(x_2+\frac{aL}{\nu}\right)^2} e^{-\frac{1}{2}\left(y_2+\frac{aL}{\nu}+bL\right)^2} \\ &\quad \frac{x_2^k H_{N+1-k}\left(\frac{aL}{\nu}\right) (y_2+bL)^l H_{N-l}\left(\frac{aL}{\nu}\right) - x_2^l H_{N-l}\left(\frac{aL}{\nu}\right) (y_2+bL)^k H_{N+1-k}\left(\frac{aL}{\nu}\right)}{x_2 - y_2 - bL}. \end{aligned}$$

One can now use another identity, which combines two Hermite polynomials with the same argument. Formula (18.18.23) from [16] is

$$H_m(x)H_n(x) = \sum_{p=0}^{\min(m,n)} \binom{m}{p} \binom{n}{p} 2^p p! H_{m+n-2p}(x).$$

We can use this to arrive at a form with only one Hermite polynomial and $y_2 + bL$ isolated. If we also introduce $c = N + 1 - k$ and $d = N - l$ we find

First matrix element of the spectral decomposition (31) with all Hermite polynomials containing the same argument

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{y}) &= C \sum_{a,b} \sum_{c=0}^{N+1} \sum_{d=0}^N \sum_{p=0}^{\max(c,d)} \binom{N+1}{N+1-c} \binom{N}{N-d} \binom{c}{p} \binom{d}{p} \\ &\quad e^{i\frac{2\pi}{L}a(x_1-y_1)} e^{-i\frac{2\pi}{L}\nu b y_1} e^{-\frac{1}{2}\left(x_2+\frac{aL}{\nu}\right)^2} e^{-\frac{1}{2}\left(y_2+\frac{aL}{\nu}+bL\right)^2} \\ &\quad \frac{x_2^{N+1-c} (y_2+bL)^{N-d} - x_2^{N-d} (y_2+bL)^{N+1-c}}{x_2 - y_2 - bL} 2^p p! H_{c+d-2p}\left(\frac{aL}{\nu}\right). \end{aligned}$$

One could also produce integrals using the following identity from [17]

$$H_n(x) = 2n \int_0^x H_{n-1}(y) dy + H_n(0),$$

which might be of benefit when correctly combined with a sum to make use of quadrature formulae.

All these forms have fewer polynomial products or beneficial arguments inside of the Hermite polynomials, but come at the expense of more sums. A possible simplification might reveal itself upon

further study. The aim of the next chapter will be to examine and verify the application of quadrature upon the spectral sum.

3.4. Quadrature tests

We now wish to check how quadrature could be applied to the spectral sum (32) with the explicit matrix elements (36), (38) and (39). The goal here is, that we want to move to a grid instead of evaluating continuous objects. In the continuum we have

$$\begin{aligned} \int_{L^2} \langle \vec{x} | i\mathcal{D} | \vec{y} \rangle \psi_m(\vec{y}) \, d^2\vec{y} &= \int_{L^2} \sum_n \lambda_n \psi_n(\vec{x}) \psi_n^\dagger(\vec{y}) \psi_m(\vec{y}) \, d^2\vec{y} \\ &= \lambda_m \psi_m(\vec{x}) \end{aligned}$$

which does not necessarily hold on discrete lattice points

$$\begin{aligned} \sum_l \langle \vec{x}_k | i\mathcal{D} | \vec{x}_l \rangle \psi_m(\vec{x}_l) &= \sum_l \sum_n \lambda_n \psi_n(\vec{x}_k) \psi_n^\dagger(\vec{x}_l) \psi_m(\vec{x}_l) \\ &= \sum_n \lambda_n \psi_n(\vec{x}_k) \sum_l \psi_n^\dagger(\vec{x}_l) \psi_m(\vec{x}_l) . \end{aligned}$$

This is where we wish to use the quadrature by choosing fitting lattice points. We already established the eigenvalue equation of the Dirac operator in chapter 2.4

$$i\mathcal{D}\varphi_{\omega,n,p} = \mu_n \varphi_{\omega,n,p}$$

and thus

$$\begin{aligned} \iiint_V \langle \vec{x} | i\mathcal{D} | \vec{y} \rangle \varphi_{\omega,n,p}(\vec{y}) \, d^3\vec{y} &= \iiint_V \sum_{m,q,\omega'} \mu_m \varphi_{\omega',m,q}(\vec{x}) \varphi_{\omega',m,q}^\dagger(\vec{y}) \varphi_{\omega,n,p}(\vec{y}) \, d^3\vec{y} \\ &= \mu_n \varphi_{\omega,n,p}(\vec{x}) , \end{aligned}$$

where V denotes the cuboid of the square L^2 and β . The key point here is the normalization of the eigenfunctions, which has already been calculated in (56). What we want to put on a grid is the expression

$$\langle \varphi_{\omega,n,p} | \varphi_{\omega',n',p'} \rangle = \delta_{\omega\omega'} \int_{L^2} \frac{1}{2\beta} \frac{1}{\sqrt{\mu(\mu-\omega)}} \frac{1}{\sqrt{\mu'(\mu'-\omega)}} \begin{pmatrix} (\mu-\omega)\varphi_{n,p}^\dagger \\ \lambda\chi_{n,p}^\dagger \end{pmatrix} \cdot \begin{pmatrix} (\mu'-\omega)\varphi_{n',p'} \\ \lambda'\chi_{n',p'} \end{pmatrix} \, d^2\vec{x}$$

or rather in the normalization of the $\varphi_{n,p}$ which are given in (22), since only this expression contains the coordinates. Their normalization has been checked in (23). Now we wish to apply the Gaussian quadrature (55) to this integral

$$\langle \varphi_{n,p} | \varphi_{m,p} \rangle = \frac{(-1)^{n+m}}{\sqrt{n!m!}\sqrt{2}^{n+m}} \int_0^L \int_0^L \varphi_{0,p}^\dagger \varphi_{0,p} \, dx \, H_n\left(\sqrt{B}y + \frac{\alpha_p}{\sqrt{B}}\right) H_m\left(\sqrt{B}y + \frac{\alpha_p}{\sqrt{B}}\right) \, dy . \quad (42)$$

The integral over x can be calculated by using (19)

$$\begin{aligned} \int_0^L \varphi_{0,p}^\dagger \varphi_{0,p} \, dx &= \sqrt{\frac{B}{\pi L^2}} \int_0^L \sum_{k \in \mathbb{Z}} \sum_{k' \in \mathbb{Z}} e^{-i(\alpha_p + kBL)x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + kL)^2} e^{i(\alpha_p + k'BL)x} e^{-\frac{B}{2}(y + \frac{\alpha_p}{B} + k'L)^2} \, dx \\ &= \sqrt{\frac{B}{\pi}} \sum_{k \in \mathbb{Z}} e^{-B(y + \frac{\alpha_p}{B} + kL)^2} . \end{aligned}$$

Thus, the former integral (42) becomes (while remembering that we have to let $\alpha_p \rightarrow \alpha_p + kBL$ in the Hermite polynomials)

$$\langle \varphi_{n,p} | \varphi_{m,p} \rangle = \frac{(-1)^{n+m}}{\sqrt{n!m!}\sqrt{2^{n+m}}} \sqrt{\frac{1}{\pi}} \int_{\mathbb{R}} e^{-y'^2} H_n(y') H_m(y') dy'$$

where we substituted $y' \equiv \sqrt{B}y + \frac{\alpha_p}{\sqrt{B}}$. Now we can apply the *Gaussian quadrature*, which is the quadrature with respect to the Hermite polynomials. A detailed account on quadrature can be found in the appendix A.2. The order of $f(x) = H_n(x)H_m(x)$ is $n + m$. Thus we have

$$\langle \varphi_{n,p} | \varphi_{m,p} \rangle = \frac{(-1)^{n+m}}{\sqrt{n!m!}\sqrt{2^{n+m}}} \sqrt{\frac{1}{\pi}} \sum_{k=1}^r \lambda_k H_n(y_k) H_m(y_k) \quad (43)$$

where the weights are the *Hermite-Gauss weights* as given in [11] as equation (25.4.46)

$$\lambda_k = \frac{2^{r-1}(r-1)!\sqrt{\pi}}{r \cdot H_{r-1}^2(y_k)}.$$

and where we need to have $r \geq \lceil \frac{n+m+1}{2} \rceil$ (where $\lceil x \rceil$ denotes x being rounded up to the nearest integer). y_k are the zeroes of H_r . For the smallest possible r this leads to

$$\langle \varphi_{n,p} | \varphi_{m,p} \rangle = \frac{1}{\sqrt{n!m!}} \begin{cases} \sum_{k=1}^{\frac{n+m}{2}+1} \frac{\frac{n+m}{2}!}{(\frac{n+m}{2}+1)H_{\frac{n+m}{2}}^2(y_k)} H_n(y_k) H_m(y_k) & , n+m \text{ even} \\ -\sum_{k=1}^{\frac{n+m+1}{2}} \frac{\sqrt{2}^{\frac{n+m+1}{2}}!}{(\frac{n+m+1}{2}+1)H_{\frac{n+m+1}{2}}^2(y_k)} H_n(y_k) H_m(y_k) & , n+m \text{ odd} . \end{cases}$$

For $n = m$ this obviously gives 1, as expected. The results of numerical calculation for the first few Hermite polynomials are in table 1.

Tab. 1: Numerical solutions of (43) for different n and m .

n \ m	0	1	2	3	4	5	6
0	1	-2.28e-17	-2.23e-15	-2.46e-17	5.82e-16	-4.17e-18	7.83e-16
1	-2.28e-17	1	-3.29e-18	-2.11e-15	-8.38e-19	2.14e-15	3.64e-18
2	-2.23e-15	-3.29e-18	1	-6.63e-19	-1.17e-16	-2.36e-18	2.94e-15
3	-2.46e-17	-2.11e-15	-6.63e-19	1	-7.26e-17	2.18e-15	-1.94e-17
4	5.82e-16	-8.38e-19	-1.17e-16	-7.26e-17	1	-0	4.77e-16
5	-4.17e-18	2.14e-15	-2.36e-18	2.18e-15	-0	1	8.93e-18
6	7.83e-16	3.64e-18	2.94e-15	-1.94e-17	4.77e-16	8.93e-18	1

We wish to also apply the quadrature after the application of Christoffel-Darboux (33). There we have, according to the calculations in appendix A.6

$$\begin{aligned} \iint_T \sum_{n=0}^N \sum_{p=1}^{\nu} \langle \varphi_{n,p} | \varphi_{n,p} \rangle d\vec{x} &= \nu \sqrt{\frac{1}{\pi}} \frac{1}{2^N N!} \int_{\mathbb{R}} \left[(N+1)H_N^2(z) - NH_{N+1}(z)H_{N-1}(z) \right] e^{-z^2} dz \\ &= \nu \sqrt{\frac{1}{\pi}} \frac{1}{2^N N!} \sum_{k=1}^r \lambda_k \left[(N+1)H_N^2(z_k) - NH_{N+1}(z_k)H_{N-1}(z_k) \right]. \end{aligned}$$

Here, the function is of order $2N$ and thus $r \geq \lceil \frac{2N+1}{2} \rceil = N+1$. So we can choose $r = N+1$, which implies that z_k are the zeroes of H_{N+1}

$$\begin{aligned} \iint_T \sum_{n=0}^N \sum_{p=1}^{\nu} \langle \varphi_{n,p} | \varphi_{n,p} \rangle d\vec{x} &= \nu \sqrt{\frac{1}{\pi}} \frac{1}{2^N N!} \sum_{k=1}^{N+1} \lambda_k \left[(N+1) H_N^2(z_k) - N \underbrace{H_{N+1}(z_k) H_{N-1}(z_k)}_{=0} \right] \\ &= \nu \sqrt{\frac{1}{\pi}} \frac{N+1}{2^N N!} \underbrace{\sum_{k=1}^{N+1} \lambda_k H_N^2(z_k)}_{=N! \sqrt{\pi} 2^N} \\ &= \nu(N+1), \end{aligned}$$

which is the expected result as in (35). Here we used, that we already verified the quadrature on Hermite polynomials. Thus, the result of $\sum_{k=1}^{N+1} \lambda_k H_N^2(z_k)$ must be the normalization weight of the Hermite polynomials.

The results of this chapter are no surprise, since the quadrature is a generally proven formula. But the interesting part is, that the quadrature leads to the possibility to compute certain integrals numerically without the intrinsic error of any integration algorithms. Also, the functions only have to be known on specific, however, in general non-equidistant, grid points.

3.5. Discretizing Space

Before, we have already found the the operator to be (32) with the explicit matrix elements (36), (38) and (39). The first direction (which has been called x at the beginning) can be discretized equidistantly, because it is given by Fourier-modes. This can be seen directly, since the operators (31) only x -dependence is located in the zero modes (19), from which the other modes (22) are constructed via ladder operators. We can choose N_x points in x -direction located at the center of a site of width L/N_x . We also wish to somehow introduce discrete coordinates in y -direction, such that we achieve simplifications via the quadrature. The appearing polynomials in the matrix elements push us to use at least the quadrature of order $N+1$.

Thus we introduce the discrete coordinates

$$\vec{x}_{skl} = \begin{pmatrix} t_s \\ x_k \\ y_l \end{pmatrix}$$

with

$$t_s \in \left\{ \frac{\beta}{N_t} \left(\frac{1}{2} + s \right) \right\}_{s \in [0, N_t]}, \quad x_k \in \left\{ \frac{L}{N_x} \left(\frac{1}{2} + k \right) \right\}_{k \in [0, N_x]}, \quad y_l \text{ related to roots of } H_{N+1}.$$

So the first matrix element (36) looks like this

$$\begin{aligned} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}_{kl}) \varphi_{n,p}^{\dagger}(\vec{x}_{k'l'}) &= \sqrt{\frac{1}{\pi L^2}} \frac{B}{2^{N+1} N!} \sum_{a,b} \frac{1}{y_l - y_{l'} - bL} \left[H_{N+1}\left(y_l + \frac{aL}{\nu}\right) H_N\left(y_{l'} + \frac{aL}{\nu} + bL\right) \right. \\ &\quad \left. - H_N\left(y_l + \frac{aL}{\nu}\right) H_{N+1}\left(y_{l'} + \frac{aL}{\nu} + bL\right) \right] \\ &\quad \cdot e^{i\frac{2\pi}{L} a(x_k - x_{k'})} e^{-i\frac{2\pi}{L} \nu b x_{k'}} e^{-\frac{1}{2}\left(y_l + \frac{aL}{\nu}\right)^2} e^{-\frac{1}{2}\left(y_{l'} + \frac{aL}{\nu} + bL\right)^2} . \end{aligned}$$

and the discrete eigenfunction (22) is

$$\varphi_{n,p}(\vec{x}_{k'l'}) = \frac{1}{\sqrt{n!}} (-1)^n \frac{1}{\sqrt{2^n}} \sum_{k \in \mathbb{Z}} H_n\left(\sqrt{B} y_{l'} + \frac{\alpha_p}{\sqrt{B}} + kBL\right) \sqrt{\frac{B}{\pi L^2}} e^{i(\alpha_p + kBL)x_{k'}} e^{-\frac{B}{2}\left(y_{l'} + \frac{\alpha_p}{B} + kL\right)^2} .$$

We need to check the following for the fully discretized version

$$\sum_{s,k,l} \langle \vec{x}_{s'l'k'l'} | i\mathcal{D} | \vec{x}_{skl} \rangle \psi_m(\vec{x}_{skl}) \Delta_{skl} = \lambda_m \psi_m(\vec{x}_{s'l'k'l'}) \quad (44)$$

where Δ_{skl} is supposed to substitute the differentials. On an equidistant grid Δ_{skl} is just the size of a grid cuboid, but since the y_l are not equidistant, Δ_{skl} is different for every l . This means we want to show that

$$\sum_{s,l,k} \psi_n^{\dagger}(\vec{x}_{slk}) \psi_m(\vec{x}_{slk}) \Delta_{skl} = \delta_{nm} .$$

For the continuum this has already been calculated in (56).

Because of the calculations in chapter 3.4 we already know that leaving the y -coordinate continuous and discretizing it implicitly by the quadrature does conserve the orthonormality and function values. They discretize analytically by the quadrature. Under the assumption, that the discretized $\varphi_{n,p}$ are orthonormal, we obviously find

$$\begin{aligned} \langle \varphi_{\omega,n,p} | \varphi_{\omega',n',p'} \rangle &= \frac{1}{2\beta} \frac{1}{\sqrt{\mu(\mu - \omega)}} \frac{1}{\sqrt{\mu'(\mu' - \omega')}} \sum_{s,k} \frac{\beta}{N_t} \frac{L}{N_x} \\ &\quad \int_0^L e^{i(\omega' - \omega)t_s} \begin{pmatrix} (\mu - \omega) \varphi_{n,p}^{\dagger} \\ \lambda \chi_{n,p}^{\dagger} \end{pmatrix} \cdot \begin{pmatrix} (\mu' - \omega') \varphi_{n',p'} \\ \lambda' \chi_{n',p'} \end{pmatrix} dy \\ &= \delta_{\omega\omega'} \delta_{nn'} \delta_{pp'} . \end{aligned}$$

So we have to check the normalization of the discretized $\varphi_{n,p}$. It is not clear, which grid points to use explicitly. The following steps try to break down, how the implicit discretization via quadrature plays out. We begin with the scalar product of of the modes $\varphi_{n,p}$ as given by (22) where t and t' are just summation indices

$$\begin{aligned} \langle \varphi_{n,p} | \varphi_{n',p'} \rangle &= \frac{(-1)^{n+n'}}{\sqrt{n!n'!2^{n+n'}}} \sum_{t,t'} \int_0^L H_n\left(\sqrt{B}(y + tL) + \frac{\alpha_p}{\sqrt{B}}\right) H_{n'}\left(\sqrt{B}(y + t'L) + \frac{\alpha_{p'}}{\sqrt{B}}\right) \\ &\quad \frac{L}{N_x} \sum_k \varphi_{0,p}^{\dagger} \varphi_{0,p'} dy , \end{aligned}$$

Conclusion

We conclude this thesis with a short summary of the results. In chapter 2, we were able to analytically solve the eigenvalue equation of the Dirac operator for fermions within a magnetic field located in a square. To achieve this, we first computed the normalized ground state of the squared Dirac operator. This squared operator allowed us to separate time and space dimensions. Then, we identified ladder operators, which allowed to write down all of the normalized modes. From there, the determination of the eigenfunctions of the Dirac operator, which are given by spinors, was possible. An extra effort has been taken to determine the zeroes of the zero modes by identification of the Jacobi theta function. We found, that the zeroes are determined by the instanton number ν and the introduced quantum number $p \leq \nu$. They are all located at the same point in the non-periodic direction and evenly spread along the periodic direction with a distance of $\frac{L}{\nu}$. This result has also been checked by application of the residue theorem.

Chapter 3 presented the discretization of the time and one periodic space dimension by application of spectral methods. For this, an expansion via Fourier series and identification of the SLAC-derivative have been used to write down a spectral sum. This expression is quite unwieldy, since every matrix element consists of four sums. By application of the Christoffel-Darboux formula this number was reduced to two. On a side note, some other expressions of the first matrix element have been computed. Then, the integrals coming up at the normalization computations have been transformed to sums via the Gaussian quadrature and the resulting expressions numerically computed to verify the applicability of a quadrature grid. Unfortunately, these considerations did not lead directly to a suitable set of grid points, because the appearing Hermite polynomials do not just include the coordinate as an argument but the coordinate shifted by a different amount for every element of the sums.

All in all, this thesis presented a few mathematical considerations which could be of interest for future attempts to find a suitable grid for the given Dirac operator. It has been tested, that the application of the Gaussian quadrature implicitly preserves the normalization of the eigenmodes. Still, this procedure did not lead directly to a suitable discretization of the non-periodic space direction. Anyway, future considerations might still benefit from some of these calculations. It might be possible to apply a Gaussian quadrature grid to a different expression of the Dirac operator, for which the considerations of chapter 3.3 might be of use. Especially a notation with Hermite polynomials with only the coordinate as an argument might prove useful. Alternatively, a different way to find a suitable grid could be connected to the zeroes of the eigenmodes. Thus, the considerations of chapter 2.3, which presents a study of the zeroes of the zero modes, might be of interest. The logical next step would be a study of the zeroes of the elevated modes. If successful, this new discretization might prove to be a useful tool in lattice field theory.

A. Appendix

A.1. Hermite polynomials

A very useful notion in mathematics is the one of orthogonality. When defining any sort of scalar product, any set of mathematical objects can be constructed to be orthogonal to each other. An example of a set of orthogonal polynomials is the one of the *Hermite polynomials*, which is well known in physics. They appear in the eigenfunctions of the quantum harmonical oscillator. Hermite polynomials are defined as those polynomials of degree n , which solve the Sturm-Liouville problem

$$\begin{aligned} H_n'' - 2xH_n' + 2nH_n &= 0 \\ \iff \partial_x(e^{-x^2}\partial_x H_n(x)) + 2ne^{-x^2}H_n(x) &= 0. \end{aligned} \quad (46)$$

Their explicit forms are

$$H_n(x) = (-1)^n e^{x^2} \partial_x^n e^{-x^2} = e^{\frac{x^2}{2}} (x - \partial_x)^n e^{-\frac{x^2}{2}} = (2x - \partial_x)^n \cdot 1, \quad (47)$$

they fulfill recursion relations

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad (48)$$

$$H_n'(x) = 2nH_{n-1}(x) \quad (49)$$

and they are orthogonal in a weighted Hilbert space with the following scalar product

$$\int_{\mathbb{R}} H_n(x)H_m(x)e^{-x^2} dx = \underbrace{2^n n! \sqrt{\pi}}_{\equiv c_n} \delta_{nm}. \quad (50)$$

With this orthonormality relation (50) and the recursion relation (49) one can show for the scalar product of their derivatives

$$\begin{aligned} \int_{\mathbb{R}} \partial_x H_n(x) \partial_x H_m(x) e^{-x^2} dx &= 4nm \int_{\mathbb{R}} H_{n-1}(x) H_{m-1}(x) e^{-x^2} dx \\ &= 4nmc_{n-1} \delta_{nm} \\ &= 4n^2 \frac{c_n}{2n} \delta_{nm} \\ &= 2nc_n \delta_{nm}. \end{aligned}$$

One can get rid of the weighting in the scalar product by defining a new set of functions containing the weight. Thus, the *Hermite functions* are defined by the Hermite polynomials as

$$\hat{H}_n(x) := e^{-\frac{x^2}{2}} H_n(x) \quad (51)$$

such that they define an orthogonal basis of $L_2(\mathbb{R})$

$$\int_{\mathbb{R}} \hat{H}_n(x) \hat{H}_m(x) dx = c_n \delta_{nm}.$$

So, since they define an orthogonal basis, we conclude that we can expand every $f(x) \in L^2(\mathbb{R})$ as

$$f(x) = \sum_n |\hat{H}_n\rangle \underbrace{\frac{1}{c_n} \langle \hat{H}_n | f \rangle}_{\equiv \hat{f}_n} = \sum_n \hat{H}_n \hat{f}_n. \quad (52)$$

With the definition of the Hermite functions (51) the Sturm-Liouville problem (46) translates to

$$\begin{aligned} & \partial_x \left[e^{-x^2} \partial_x e^{\frac{x^2}{2}} \hat{H}_n(x) \right] + 2n e^{-x^2} e^{\frac{x^2}{2}} \hat{H}_n(x) = 0 \\ \iff & \partial_x \left[x e^{-x^2} e^{\frac{x^2}{2}} \hat{H}_n(x) + e^{-x^2} e^{\frac{x^2}{2}} \partial_x \hat{H}_n(x) \right] + 2n e^{-\frac{x^2}{2}} \hat{H}_n(x) = 0 \quad | \cdot e^{\frac{x^2}{2}} \\ \iff & e^{\frac{x^2}{2}} \partial_x \left[x e^{-\frac{x^2}{2}} \hat{H}_n(x) + e^{-\frac{x^2}{2}} \partial_x \hat{H}_n(x) \right] + 2n \hat{H}_n(x) = 0. \end{aligned}$$

The recursion relations (48) and (49) translate to

$$\begin{aligned} e^{\frac{x^2}{2}} \hat{H}_{n+1}(x) &= 2x e^{\frac{x^2}{2}} \hat{H}_n(x) - 2n e^{\frac{x^2}{2}} \hat{H}_{n-1}(x) \\ \iff \hat{H}_{n+1}(x) &= 2x \hat{H}_n(x) - 2n \hat{H}_{n-1}(x) \end{aligned} \tag{53}$$

and

$$\begin{aligned} \partial_x e^{\frac{x^2}{2}} \hat{H}_n(x) &= 2n e^{\frac{x^2}{2}} \hat{H}_{n-1}(x) \\ \iff \cancel{e^{\frac{x^2}{2}}} \partial_x \hat{H}_n(x) + \cancel{e^{\frac{x^2}{2}}} x \hat{H}_n(x) &= 2n \cancel{e^{\frac{x^2}{2}}} \hat{H}_{n-1}(x) \\ \stackrel{(53)}{\iff} \hat{H}'_n(x) &= n \hat{H}_{n-1}(x) - \frac{1}{2} \hat{H}_{n+1}(x). \end{aligned}$$

Here are three more useful identities of the Hermite polynomials and Hermite functions

$$\begin{aligned} \int_0^x H_n(y) \, dy &= \frac{1}{2(n+1)} [H_{n+1}(x) - H_{n+1}(0)] \\ \int_0^x e^{-y^2} H_n(y) \, dy &= H_{n-1}(0) - e^{-x^2} H_{n+1}(x) \\ \int_{\mathbb{R}} \hat{H}'_n(x) \hat{H}'_m(x) \, dx &= \begin{cases} n^2 c_{n-1} + \frac{1}{4} c_{n+1} & , n = m \\ -\frac{n}{2} c_{n-1} & , m = n - 2 \\ -\frac{n+2}{2} c_{n+1} & , m = n + 2 \end{cases} \end{aligned}$$

Also, because of (52), one can introduce $N + 1$ -dimensional subspaces

$$\mathcal{H}_N = \text{span}\{\hat{H}_0(x), \hat{H}_1(x), \dots, \hat{H}_N(x)\} \subset L^2(\mathbb{R})$$

on which orthogonal projections $P_N : L^2(\mathbb{R}) \mapsto \mathcal{H}_N$ are given by

$$(P_N f)(x) = \sum_{n=0}^N \hat{f}_n \hat{H}_n(x).$$

A.2. Quadrature

The biggest issue in numerical mathematics is the one of error. Any computation done by a machine carries an error with it, which can become quite problematic when using algorithms containing a large number of computations, especially multiplications. For orthogonal polynomials, such as the Hermite polynomials presented in the former chapter, there is a powerful application called *quadrature*. The technique allows for (weighted) integrals of polynomials to be exchanged by (weighted) finite sums, which only have to be evaluated at the zeroes of certain orthogonal polynomials. This is useful, because the numerical evaluation of integrals requires a discretization anyway, which normally leads to a discretization error depending on the chosen step width. But quadrature substitutes integrals by

sums analytically, which avoids this error entirely. To understand the nature of this statement, we now go on to derive and prove it.

Let $x_1 < x_2 < \dots < x_n$ be the ordered zeroes of the polynomial $p_n(x) \prod_{k=1}^n (x - x_k)$. The *Lagrange interpolation polynomial*

$$l_k(x) = \frac{\prod_{j,j \neq k} (x - x_j)}{\prod_{j,j \neq k} (x_k - x_j)}$$

is the unique polynomial of degree $< n$ such that $l_k(x_j) = \delta_{kj}$ for $j = 1, 2, \dots, n$. This way we can expand any polynomial r of degree $< n$ as

$$r(x) = \sum_{k=1}^n r(x_k) l_k(x). \quad (54)$$

Now we are ready to prove the following statements:

Gaussian quadrature

Let p_n be an orthogonal polynomial of order n with respect to to weighting function μ and let l_k be the Lagrange interpolation polynomials associated with the zeros x_1, \dots, x_n of p_n . Define

$$\lambda_k := \int_{\mathbb{R}} l_k(x) \, d\mu(x).$$

Then for all polynomials $f(x)$ of degree $\leq 2n - 1$ we have

$$\int_{\mathbb{R}} f(x) \, d\mu(x) = \sum_{k=1}^n \lambda_k f(x_k) \quad \text{and} \quad \lambda_k = \int_{\mathbb{R}} l_k^2(x) \, d\mu(x) > 0. \quad (55)$$

To prove the first statement we assume f to be a polynomial of degree $\leq 2n - 1$. By theory of polynomial division we can find polynomials q and r of degree $\leq n - 1$ such that $f(x) = q(x)p_n(x) + r(x)$. At the roots of p_n we obviously have $f(x_k) = r(x_k)$. Thus we have

$$\int_{\mathbb{R}} f(x) \, d\mu(x) = \int_{\mathbb{R}} q(x)p_n(x) \, d\mu(x) + \int_{\mathbb{R}} r(x) \, d\mu(x).$$

The first integral just gives zero, since q is just a linear combination of p_k with $k \leq n - 1$ and those are orthonormal with respect to μ . So with the use of (54) we find

$$\begin{aligned} \int_{\mathbb{R}} f(x) \, d\mu(x) &= \int_{\mathbb{R}} r(x) \, d\mu(x) \\ &= \sum_{k=1}^n r(x_k) \int_{\mathbb{R}} l_k(x) \, d\mu(x) \\ &= \sum_{k=1}^n f(x_k) \lambda_k. \end{aligned}$$

We can use this to prove the second relation

$$\begin{aligned} \int_{\mathbb{R}} l_k^2(x) \, d\mu(x) &= \sum_{j=1}^n l_k^2(x_j) \lambda_j \\ &= \sum_{j=1}^n \delta_{kj} \lambda_j \\ &= \lambda_k. \quad \square \end{aligned}$$

Having a tool at hand to substitute integrals over the whole real axis by finite sums at specific points can prove very useful whenever the functions of interest happen to be polynomials.

A.3. Normalization checks

The following is an explicit verification of the normalization of the alternative representation of the eigenmodes (24) of the squared Dirac operator (8). We compute the scalar product $\langle \varphi_{n,p} | \varphi_{m,q} \rangle$, to check the normalization

$$\begin{aligned}
\langle \varphi_{n,p} | \varphi_{m,q} \rangle &= \frac{(-1)^n}{\sqrt{2^n n!}} \frac{(-1)^m}{\sqrt{2^m m!}} \sqrt{\frac{B}{\pi L^2}} \int_0^L \sum_{k,k'} \hat{H}_n(p, k) \hat{H}_m(q, k') \underbrace{\int_0^L e^{2\pi i [q-p+(k'-k)\nu] \frac{x}{L}} dx}_{=L\delta_{pq}\delta_{kk'}} dy \\
&= \delta_{pq} \frac{(-1)^{m+n}}{\sqrt{2^{m+n} n! m!}} \sqrt{\frac{B}{\pi}} \sum_{k \in \mathbb{Z}} \int_0^L \hat{H}_n\left(\sqrt{\Phi}\left(\frac{y}{L} + \frac{p+k\nu}{\nu}\right)\right) \hat{H}_m\left(\sqrt{\Phi}\left(\frac{y}{L} + \frac{p+k\nu}{\nu}\right)\right) dy \\
&= \delta_{pq} \frac{(-1)^{m+n}}{\sqrt{2^{m+n} n! m!}} \sqrt{\frac{B}{\pi}} \sum_{k \in \mathbb{Z}} \int_0^L \hat{H}_n\left(\sqrt{B}\left(y + kL + \frac{p}{\nu}\right)\right) \hat{H}_m\left(\sqrt{B}\left(y + kL + \frac{p}{\nu}\right)\right) dy \\
&= \delta_{pq} \frac{(-1)^{m+n}}{\sqrt{2^{m+n} n! m!}} \sqrt{\frac{B}{\pi}} \int_{\mathbb{R}} \hat{H}_n(\sqrt{B}y) \hat{H}_m(\sqrt{B}y) dy \\
&= \delta_{pq} \frac{(-1)^{m+n}}{\sqrt{2^{m+n} n! m!}} \sqrt{\frac{\beta}{\pi}} \int_{\mathbb{R}} \hat{H}_n(z) \hat{H}_m(z) \frac{dz}{\sqrt{\beta}} \\
&= \delta_{pq} \frac{(-1)^{m+n}}{\sqrt{2^{m+n} n! m!} \pi} 2^n n! \sqrt{\pi} \delta_{nm} \\
&= \delta_{pq} \delta_{nm} \underbrace{(-1)^{2n}}_{=1}.
\end{aligned}$$

Now comes a check of the eigenmodes (22) of the original Dirac operator (7)

$$\begin{aligned}
\langle \varphi_{\omega, n, p} | \varphi_{\omega', n', p'} \rangle &= \frac{1}{2\beta} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \frac{1}{\sqrt{\mu_{n'}(\mu_{n'} - \omega')}} \iiint_V e^{i(\omega' - \omega)x^0} \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p}^\dagger \\ \lambda_n \chi_{n,p}^\dagger \end{pmatrix} \cdot \begin{pmatrix} (\mu_{n'} - \omega')\varphi_{n',p'} \\ \lambda_{n'} \chi_{n',p'} \end{pmatrix} dV \\
&= \frac{1}{2\beta} \frac{1}{\sqrt{\mu_n(\mu_n - \omega)}} \frac{1}{\sqrt{\mu_{n'}(\mu_{n'} - \omega')}} \delta_{\omega\omega'} \beta \int_0^L \int_0^L \begin{pmatrix} (\mu_n - \omega)\varphi_{n,p}^\dagger \\ \lambda_n \chi_{n,p}^\dagger \end{pmatrix} \cdot \begin{pmatrix} (\mu_{n'} - \omega)\varphi_{n',p'} \\ \lambda_{n'} \chi_{n',p'} \end{pmatrix} dx dy \\
&= \frac{1}{2} \frac{1}{\mu_n(\mu_n - \omega)} \delta_{\omega\omega'} \delta_{nn'} \delta_{pp'} \begin{pmatrix} \mu_n - \omega \\ \lambda_n \end{pmatrix} \cdot \begin{pmatrix} \mu_n - \omega \\ \lambda_n \end{pmatrix} \\
&= \frac{1}{2} \frac{\mu_n^2 - 2\mu_n\omega + \omega^2 + \lambda_n^2}{\mu_n(\mu_n - \omega)} \delta_{\omega\omega'} \delta_{nn'} \delta_{pp'} \tag{56} \\
&= \frac{\mu_n^2 - \mu_n\omega}{\mu_n(\mu_n - \omega)} \delta_{\omega\omega'} \delta_{nn'} \delta_{pp'} \\
&= \delta_{\omega\omega'} \delta_{nn'} \delta_{pp'}.
\end{aligned}$$

A.4. Jacobi theta function

The Jacobi theta function comes up when searching for a non constant entire complex function which is invariant on a lattice generated by 1 and τ . When following the thoughts in [12], this leads to the definition of the Jacobi theta function

$$\vartheta(z, \tau) := \sum_{k \in \mathbb{Z}} e^{\pi i k^2 \tau + 2\pi i k z}$$

for $z \in \mathbb{C}$ and $\tau \in \{w \in \mathbb{C} | \Im w > 0\}$. Let us consider τ to be a constant, such that we can study the periodic behavior in z . This function obviously has the period 1. With respect to τ it has the quasi-periodic behaviour

$$\vartheta(z + \tau, \tau) = e^{-\pi i \tau - 2\pi i z} \vartheta(z, \tau) .$$

In the scope of this work, but also generally in mathematics, we are interested in the zeroes of this function. Those are given by

$$z_{mn} = \left(m + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right)\tau, \quad m, n \in \mathbb{Z} . \quad (57)$$

This can be checked by using the periodic behavior of the function

$$\begin{aligned} \vartheta(z_{mn}, \tau) &= \vartheta\left[\left(m + \frac{1}{2}\right) + \left(n + \frac{1}{2}\right)\tau, \tau\right] \\ &= e^{-n\pi i \tau - 2n\pi i z} \vartheta\left[\frac{1}{2} + \frac{1}{2}\tau, \tau\right] \\ &= e^{-n\pi i \tau - 2n\pi i z} \sum_{k \in \mathbb{Z}} e^{\pi i k^2 \tau + \pi i k(1+\tau)} \\ &= e^{-n\pi i \tau - 2n\pi i z} \sum_{k \in \mathbb{Z}} (-1)^k e^{\pi i (k^2 + k)\tau} \\ &= e^{-n\pi i \tau - 2n\pi i z} \left[\sum_{k \in \mathbb{N}_0} (-1)^k e^{\pi i (k^2 + k)\tau} + \sum_{k=-1}^{-\infty} (-1)^k e^{\pi i (k^2 + k)\tau} \right] \\ &= e^{-n\pi i \tau - 2n\pi i z} \left[\sum_{k \in \mathbb{N}_0} (-1)^k e^{\pi i (k^2 + k)\tau} + \sum_{k \in \mathbb{N}_0} (-1)^{-(k+1)} e^{\pi i [(k+1)^2 - k - 1]\tau} \right] \\ &= e^{-n\pi i \tau - 2n\pi i z} \sum_{k \in \mathbb{N}_0} \underbrace{\left[(-1)^k + (-1)^{k+1} \right]}_{=0} e^{\pi i (k^2 + k)\tau} \\ &= 0 . \end{aligned}$$

A.5. Verification of the zeroes of the zero modes via residue theorem

With the residue theorem one can find the number of zeroes and poles of a function f on a simply connected area V on the complex plane by evaluating the line integral along its boundary γ . More explicitly, for a function with no poles and no zeroes on the contour we have for the amount of zeroes n enclosed by γ

$$n = \frac{1}{2\pi i} \oint_{\gamma} \frac{f'(z)}{f(z)} dz. \quad (58)$$

Since the modes have no poles, the amount of zeroes can be found via this integral. But we have to exclude the case $p = \frac{\nu}{2}$, since in that case the zeroes would be located along γ .

When considering the zero modes as given by (19), we realize that the factor outside of the sum never vanishes. Thus, we only have to look for the zeroes of the sum. When also introducing the complex coordinate $z = -y + ix \equiv x' + iy'$, we want to determine the zeroes of

$$f(z) = \sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(BLz + \alpha_p L)} .$$

To compute the derivative, we use the approach of the Cauchy-Riemann equations. The statement is, that the derivative of the complex function

$$f(z) = u(x', y') + iv(x', y')$$

with respect to z is given by the derivatives $u_x := \partial_x u$

$$f'(z) = u_{x'} + iv_{x'} = v_{y'} - iu_{y'}.$$

The appearing identities $u_{x'} = v_{y'}$ and $v_{x'} = -u_{y'}$ are known as the *Cauchy-Riemann differential equations*. If they are fulfilled, the function is complex differentiable. So first we need to determine $u(x', y')$ and $v(x', y')$

$$\begin{aligned} f(z) &= \sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(BLz + \alpha_p L)} \\ &= \sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} e^{ikBLy'} \\ &= i \underbrace{\sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \sin(kBLy')}_{=v(x', y')} + \\ &\quad \underbrace{\sum_{k \in \mathbb{Z}} e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \cos(kBLy')}_{=u(x', y')}. \end{aligned}$$

The derivatives of u and v are then simply calculated to be

$$\begin{aligned} u_{x'}(x', y') &= BL \sum_{k \in \mathbb{Z}} k e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \cos(kBLy') \\ v_{x'}(x', y') &= BL \sum_{k \in \mathbb{Z}} k e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \sin(kBLy') \\ u_{y'}(x', y') &= -BL \sum_{k \in \mathbb{Z}} k e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \sin(kBLy') \\ v_{y'}(x', y') &= BL \sum_{k \in \mathbb{Z}} k e^{-k^2 \frac{BL^2}{2} + k(BLx' + \alpha_p L)} \cos(kBLy'). \end{aligned}$$

Those obviously fulfill the Cauchy-Riemann differential equations. Thus, the derivative is given by

$$f'(z) = \sum_{k \in \mathbb{Z}} kBL e^{-k^2 \frac{BL^2}{2} + k(BLz + \alpha_p L)}.$$

The integration contour around the area of interest can be seen in figures 3 and 4.

Since both f and f' are periodic in $y' \mapsto y' + L$, the integral reduces to

$$\oint_{\gamma} \frac{f'(z)}{f(z)} dz = \int_0^L \frac{f'(0, y')}{f(0, y')} idy' + \int_L^0 \frac{f'(-L, y')}{f(-L, y')} idy'.$$

To solve the integral we separate imaginary and real parts

$$\begin{aligned} \oint_{\gamma} \frac{f'(z)}{f(z)} dz &= \oint_{\gamma} \frac{\Re f' + i\Im f'}{\Re f + i\Im f} dz \\ &= \oint_{\gamma} \frac{(\Re f' + i\Im f')(\Re f - i\Im f)}{\Re^2 f + \Im^2 f} dz \\ &= \oint_{\gamma} \frac{\Re f' \Re f + \Im f' \Im f}{\Re^2 f + \Im^2 f} dz + i \oint_{\gamma} \frac{\Im f' \Re f - \Re f' \Im f}{\Re^2 f + \Im^2 f} dz. \end{aligned}$$

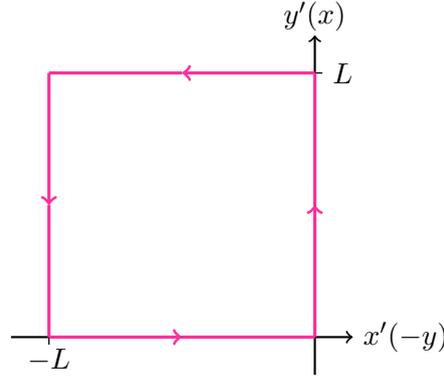


Fig. 3: Integral contour used to find the amount of zeroes in the newly defined complex coordinates.

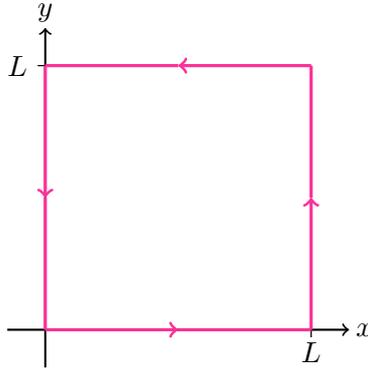


Fig. 4: Integral contour used to find the amount of zeroes in the original coordinates.

For the real part we get

$$\begin{aligned}
& \oint_{\gamma} \frac{\sum_{k,k'} kBL e^{-(k^2+k'^2)\frac{BL^2}{2}+(k+k')(\alpha_p L+BLx')} \left[\cos(kBLy') \cos(k'BLy') + \sin(kBLy') \sin(k'BLy') \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\frac{BL^2}{2}+(n+n')(\alpha_p L+BLx')} \left[\cos(nBLy') \cos(n'BLy') + \sin(nBLy') \sin(n'BLy') \right]} dz \\
&= \oint_{\gamma} \frac{\sum_{k,k'} kBL e^{-(k^2+k'^2)\frac{BL^2}{2}+(k+k')(\alpha_p L+BLx')} \cos \left[(k-k')BLy' \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\frac{BL^2}{2}+(n+n')(\alpha_p L+BLx')} \cos \left[(n-n')BLy' \right]} dz \\
&= \oint_{\gamma} \frac{\sum_{k,k'} \frac{2\pi\nu k}{L} e^{-(k^2+k'^2)\pi\nu+2\pi(k+k')\left(p+\nu\frac{x'}{L}\right)} \cos \left[2\pi\nu(k-k')\frac{y'}{L} \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\pi\nu+2\pi(n+n')\left(p+\nu\frac{x'}{L}\right)} \cos \left[2\pi\nu(n-n')\frac{y'}{L} \right]} dz.
\end{aligned}$$

Numerical calculation leads to the following result with an accuracy of 13 digits

$$\oint_{\gamma} \frac{\Re f' \Re f + \Im f' \Im f}{\Re^2 f + \Im^2 f} dz = i2\pi\nu, \quad p \neq \frac{\nu}{2}.$$

For the imaginary part we get

$$\begin{aligned}
& \oint_{\gamma} \frac{\sum_{k,k'} kBL e^{-(k^2+k'^2)\frac{BL^2}{2}+(k+k')(\alpha_p L+BLx')} \left[\sin(kBLy') \cos(k'BLy') - \cos(kBLy') \sin(k'BLy') \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\frac{BL^2}{2}+(n+n')(\alpha_p L+BLx')} \cos \left[(n-n')BLy' \right]} dz \\
&= \oint_{\gamma} \frac{\sum_{k,k'} kBL e^{-(k^2+k'^2)\frac{BL^2}{2}+(k+k')(\alpha_p L+BLx')} \sin \left[(k-k')BLy' \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\frac{BL^2}{2}+(n+n')(\alpha_p L+BLx')} \cos \left[(n-n')BLy' \right]} dz \\
&= \oint_{\gamma} \frac{\sum_{k,k'} \frac{2\pi\nu k}{L} e^{-(k^2+k'^2)\pi\nu+2\pi(k+k')(p+\nu\frac{x'}{L})} \sin \left[2\pi\nu(k-k')\frac{y'}{L} \right]}{\sum_{n,n'} e^{-(n^2+n'^2)\pi\nu+2\pi(n+n')(p+\nu\frac{x'}{L})} \cos \left[2\pi\nu(n-n')\frac{y'}{L} \right]} dz.
\end{aligned}$$

Again, numerical calculation leads to the result that this integral vanishes up to an accuracy of 25 digits. Thus, the complete result for the integral is

$$\oint_{\gamma} \frac{f'(z)}{f(z)} dz = i2\pi\nu, \quad p \neq \frac{\nu}{2}.$$

When comparing with the residue theorem (58) we find the expected result

$$n = \frac{1}{2\pi i} \oint_{\gamma} \frac{f'(z)}{f(z)} dz = \nu.$$

A.6. Verification of the first matrix element after application of Christoffel-Darboux

Here we wish to check the result (34). For this we consider the special case $\vec{x} = \vec{y}$

$$\begin{aligned}
\sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{x}) &= \sqrt{\frac{1}{\pi L^2}} \sum_{a,b} \frac{1}{2^{N+1} N!} \frac{1}{-bL} \left\{ H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} + bL \right) \right] \right. \\
&\quad \left. - H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} + bL \right) \right] \right\} \\
&\quad \cdot e^{-i\frac{2\pi}{L}\nu b x_1} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} \right)^2} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} + bL \right)^2}
\end{aligned}$$

where only terms with $b = 0$ contribute to the integral over x_1

$$\begin{aligned}
\int_0^L \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{x}) \, dx_1 &= \lim_{b \rightarrow 0} \int_0^L \sqrt{\frac{1}{\pi L^2}} \sum_a \frac{1}{2^{N+1} N!} \frac{1}{bL} \\
&\quad \cdot \left\{ H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} + bL \right) \right] \right. \\
&\quad \left. - H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} + bL \right) \right] \right\} \\
&\quad \cdot e^{-i \frac{2\pi}{L} \nu b x_1} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} \right)^2} e^{-\frac{B}{2} \left(x_2 + \frac{aL}{\nu} + bL \right)^2} \, dx_1 \\
&= \sqrt{\frac{B}{\pi L^2}} \sum_a \frac{1}{2^{N+1} N!} \\
&\quad \cdot \left\{ H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H'_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] \right. \\
&\quad \left. - H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H'_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] \right\} \\
&\quad \cdot e^{-B \left(x_2 + \frac{aL}{\nu} \right)^2} \int_0^L dx_1.
\end{aligned}$$

When also integrating over x_2 we can use the identity

$$\sum_a \int_0^L f \left(x + \frac{aL}{\nu} \right) \, dx = \nu \int_{\mathbb{R}} f(x) \, dx$$

to get

$$\begin{aligned}
\int_{L^2} \sum_{n=0}^N \sum_{p=1}^{\nu} \varphi_{n,p}(\vec{x}) \varphi_{n,p}^{\dagger}(\vec{x}) \, d\vec{x} &= \int_0^L \sqrt{\frac{B}{\pi}} \sum_a \frac{1}{2^{N+1} N!} \\
&\quad \cdot \left\{ H_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H'_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] \right. \\
&\quad \left. - H_{N+1} \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] H'_N \left[\sqrt{B} \left(x_2 + \frac{aL}{\nu} \right) \right] \right\} \\
&\quad \cdot e^{-B \left(x_2 + \frac{aL}{\nu} \right)^2} \, dx_2 \\
&= \nu \sqrt{\frac{B}{\pi}} \frac{1}{2^{N+1} N!} \int_{\mathbb{R}} \left[H_N(\sqrt{B}x_2) H'_{N+1}(\sqrt{B}x_2) \right. \\
&\quad \left. - H_{N+1}(\sqrt{B}x_2) H'_N(\sqrt{B}x_2) \right] e^{-Bx_2^2} \, dx_2 \\
&= \nu \sqrt{\frac{B}{\pi}} \frac{1}{2^N N!} \int_{\mathbb{R}} \left[(N+1) H_N^2(\sqrt{B}x_2) \right. \\
&\quad \left. - N H_{N+1}(\sqrt{B}x_2) H_{N-1}(\sqrt{B}x_2) \right] e^{-Bx_2^2} \, dx_2 \\
&= \nu \sqrt{\frac{1}{\pi}} \frac{1}{2^N N!} \int_{\mathbb{R}} \left[(N+1) H_N^2(z) - N H_{N+1}(z) H_{N-1}(z) \right] e^{-z^2} \, dz \\
&= \nu(N+1)
\end{aligned}$$

Bibliography

- [1] Andreas Wipf. *Statistical Approach to Quantum Field Theory*. Vol. 864. Jan. 2013. ISBN: 978-3-642-33104-6. DOI: 10.1007/978-3-642-33105-3.
- [2] Julian J. Lenz, Michael Mandl, and Andreas Wipf. “Magnetic catalysis in the (2+1)-dimensional Gross-Neveu model”. In: *Phys. Rev. D* 107 (9 May 2023), p. 094505. DOI: 10.1103/PhysRevD.107.094505. URL: <https://link.aps.org/doi/10.1103/PhysRevD.107.094505>.
- [3] Shu Nakamura. *Remarks on discrete Dirac operators and their continuum limits*. 2023. arXiv: 2306.14180 [math-ph].
- [4] R. Narayanan. *Tata lectures on overlap fermions*. 2011. arXiv: 1103.4588 [hep-lat].
- [5] Pavlos M. Vranas. “Gap domain wall fermions”. In: *Phys. Rev. D* 74 (3 2006), p. 034512. DOI: 10.1103/PhysRevD.74.034512. URL: <https://link.aps.org/doi/10.1103/PhysRevD.74.034512>.
- [6] Rajan Gupta. *Introduction to Lattice QCD*. 1998. arXiv: hep-lat/9807028 [hep-lat].
- [7] Tom H. Koornwinder. “Orthogonal Polynomials”. In: *Computer Algebra in Quantum Field Theory*. Springer Vienna, 2013, pp. 145–170. ISBN: 9783709116166. DOI: 10.1007/978-3-7091-1616-6_6. URL: http://dx.doi.org/10.1007/978-3-7091-1616-6_6.
- [8] Martin Hermann. *Numerische Mathematik*. München: Oldenbourg Wissenschaftsverlag, 2011. ISBN: 9783486719703. DOI: doi:10.1524/9783486708202. URL: <https://doi.org/10.1524/9783486708202>.
- [9] *Quantenfeldtheorie, Vorlesungsskriptum*. 2020. URL: <http://www.tpi.uni-jena.de/qfphysics/homepage/wipf/lectures/qft1/qft1head.pdf>.
- [10] Ivo Sachs and Andreas Wipf. *Finite Temperature Schwinger Model*. 2010. arXiv: 1005.1822 [hep-th].
- [11] Milton Abramowitz and Irene A Stegun. *Handbook of mathematical functions with formulas, graphs, and mathematical tables*. Vol. 55. US Government printing office, 1968.
- [12] Simon Rubinstein-Salzedo. *The Jacobi ϑ Function*. 2005. URL: <http://simonrs.com/JacobiTheta.pdf>.
- [13] Sidney D. Drell, Marvin Weinstein, and Shimon Yankielowicz. “Strong-coupling field theory. I. Variational approach to φ^4 theory”. In: *Phys. Rev. D* 14 (2 1976), pp. 487–516. DOI: 10.1103/PhysRevD.14.487. URL: <https://link.aps.org/doi/10.1103/PhysRevD.14.487>.
- [14] Sidney D. Drell, Marvin Weinstein, and Shimon Yankielowicz. “Strong-coupling field theories. II. Fermions and gauge fields on a lattice”. In: *Phys. Rev. D* 14 (6 1976), pp. 1627–1647. DOI: 10.1103/PhysRevD.14.1627. URL: <https://link.aps.org/doi/10.1103/PhysRevD.14.1627>.
- [15] Zhi-yuan Huang and Jia-an Yan. “Foundations of Infinite Dimensional Analysis”. In: *Introduction to Infinite Dimensional Stochastic Analysis*. Dordrecht: Springer Netherlands, 2000. ISBN: 978-94-011-4108-6. DOI: 10.1007/978-94-011-4108-6_1. URL: https://doi.org/10.1007/978-94-011-4108-6_1.
- [16] Frank Olver et al. *The NIST Handbook of Mathematical Functions*. en. Cambridge University Press, New York, NY, 2010.

- [17] Harry Bateman and Bateman Manuscript Project. *Higher Transcendental Functions [Volume II]*. Funding by Office of Naval Research (ONR). McGraw-Hill Book Company, 1953.

Eidesstattliche Erklärung

Ich erkläre hiermit, dass ich die vorliegende Arbeit selbstständig, ohne weitere Hilfsmittel als angegeben und ohne Verwendung einer generierenden KI-Anwendung angefertigt habe. Die eingereichte Arbeit ist nicht anderweitig als Prüfungsleistung verwendet worden oder in deutscher oder einer anderen Sprache als Veröffentlichung erschienen. Seitens des Verfassers bestehen keine Einwände, die vorliegende Bachelorarbeit für die öffentliche Benutzung zur Verfügung zu stellen.

Jena, 24. März 2024

Vladislav Guschakowski

Danksagung

Ich möchte mich an dieser Stelle bei meinen Betreuern für eine lehrreiche und angenehme Zusammenarbeit bedanken.

Prof. Andreas Wipf danke ich für die Möglichkeit, mich bereits in der Bachelorarbeit mit einem solch interessanten und komplexen Thema befassen zu dürfen. Ich schätze durchaus die vielen, zeitintensiven Diskussionen der Rechnungen und die zahllosen Hilfestellungen. Vor allem danke ich Ihnen für ihre Geduld.

Dr. Michael Mandl danke ich für die umfassende Einführung in die Quantenfeldtheorie, welche mir den Einstieg in dieses Thema überhaupt erst ermöglicht hat. Besonders zu schätzen weiß ich das ausführliche Feedback, das Nachrechnen der zahlreichen Rechnungen und sehr wertvolle Hinweise zu Inhalt und Struktur.