Contents

1 Basics on superstring theory

In this chapter we want to give a brief introduction to the basic concepts of string theory, starting from its simplest possible form, the bosonic string and further develop the subject to a supersymmetric version including fermions. Since we want to apply the concepts of AdS/CFT, we are mostly interested in strings propagating in AdS backgrounds. The following assertions are mainly based on the remarks in [1, 2, 3].

1.1 The bosonic string

The basic idea of string theory is that the fundamental objects described by the theory are extended from point-like particles to one-dimensional strings propagating through spacetime and sweeping out a $(1+1)$-dimensional surface $\widetilde{\Sigma}$ called the string worldsheet. The string can be parameterized by two coordinates, the proper time τ and the spatial extent σ of the string which we will also denote by $(\sigma^0, \sigma^1) = (\tau, \sigma)$. We can then apply a homeomorphism $\big(\Sigma, \phi\big)$ that maps the 2d sheet Σ into the target space which is a D-dimensional MINKOWSKI space[1] $\mathbb{R}^{D-1,1}$ with embedding coordinates $X^\mu(\tau, \sigma)$ and therefore

$$\begin{array}{rccl} \phi: & \Sigma = (\tau_{\text{in}}, \tau_{\text{fin}}) \times (0, \sigma) & \longrightarrow & \widetilde{\Sigma} \\ & (\tau, \sigma) & \longrightarrow & X^\mu(\tau, \sigma). \end{array} \tag{1.1.1}$$

The simplest possible action is proportional to the area of the surface of $\widetilde{\Sigma}$, given by

$$S_{\text{NG}} = -\frac{1}{2\pi\alpha'} \int\limits_{\Sigma} \mathrm{d}^2\sigma \, \sqrt{-\gamma}, \tag{1.1.2}$$

where γ is the GRAMIAN determinant of the embedding

$$\gamma = \det\big(\gamma_{\alpha\beta}\big), \quad \gamma_{\alpha\beta} = \partial_\alpha X^M \partial_\beta X^N \eta_{MN}, \quad \partial_\alpha \equiv \frac{\partial}{\partial\sigma^\alpha}, \quad \alpha = 0, 1\ , \tag{1.1.3}$$

where the induced metric $\gamma_{\alpha\beta}$ is the pull-back of the flat MINKOWSKI metric η_{MN}. We also defined $\mathrm{d}^2\sigma = \mathrm{d}\sigma^0 \mathrm{d}\sigma^1$ and the parameter in front of the integral is the string tension, making the action dimensionless, with the Regge slope α' being related to the string length l_{s} by $\alpha' = l_{\text{s}}^2$. Due to the

[1] We will utilize the metric $\eta_{MN} = \text{diag}(-, +, +, \ldots, +)$ with $M, N = 0, 1, 2, \ldots, D-1$.

square root this so called NAMBU-GOTO action is not very suitable for a path integral quantization. To get rid of the square root one can introduce an auxiliary metric $h_{\alpha\beta}(\sigma)$ with $h_{\alpha\beta}h^{\beta\rho} = \delta^\rho_\alpha$ and define the POLYAKOV action by

$$S_{\mathrm{P}} = -\frac{1}{4\pi\alpha'}\int_\Sigma \mathrm{d}^2\sigma\,\sqrt{-h}h^{\alpha\beta}\gamma_{\alpha\beta}. \tag{1.1.4}$$

This action is equivalent to the NAMBU-GOTO action on the classical level which can be proved by deriving the equations of motion for $h_{\alpha\beta}$, $\delta S/\delta h^{\alpha\beta} = 0$. We can use this to define the corresponding energy-momentum tensor

$$T_{\alpha\beta} \equiv -4\pi\alpha'\frac{1}{\sqrt{-h}}\frac{\delta S}{\delta h^{\alpha\beta}} = \gamma_{\alpha\beta} - \frac{1}{2}h_{\alpha\beta}h^{\rho\sigma}\gamma_{\rho\sigma} = 0. \tag{1.1.5}$$

From the constraint that $T_{\alpha\beta}$ has to vanish we can derive the classical equivalence of the actions S_{NG} and S_{P} with

$$\sqrt{-\gamma} = \frac{1}{2}\sqrt{-h}h^{\rho\sigma}\gamma_{\rho\sigma}. \tag{1.1.6}$$

We will thus use the the POLYAKOV action in the following, since it is easier to handle. But before we continue, we want to analyse the symmetries preserved by the POLYAKOV action.

- *Global D-dimensional Poincarè invariance*

  $$X^M \to \widetilde{X}^M = \Lambda^M_N X^N + a^M, \qquad \delta h_{\alpha\beta} = 0, \tag{1.1.7}$$

  with Λ^M_N and a^M being D-dimensional LORENTZ transformations and spacetime translations.

- *Reparametrisation invariance of the worldsheet (or diffeomorphism invariance)*

  We can choose a reparametrisation of the worldsheet coordinates $\sigma^\alpha \to \tilde{\sigma}^\alpha(\sigma)$, where the fields X^M and the 2d metric transform according

  $$\begin{aligned} X^M(\sigma) &\to \widetilde{X}^M(\tilde{\sigma}) = X^M(\sigma), \\ h_{\alpha\beta}(\sigma) &\to \tilde{h}_{\alpha\beta}(\tilde{\sigma}) = \frac{\partial\sigma^\alpha}{\partial\tilde{\sigma}^\gamma}\frac{\partial\sigma^\beta}{\partial\tilde{\sigma}^\delta}h_{\gamma\delta}(\sigma). \end{aligned} \tag{1.1.8}$$

  This is a gauge symmetry on the worldsheet.

- *Weyl invariance*

  $$\widetilde{X}^M(\sigma) = X^M(\sigma), \qquad \tilde{h}_{\alpha\beta}(\sigma) = \Omega^2 h_{\alpha\beta}(\sigma). \tag{1.1.9}$$

We also have to employ suitable boundary conditions. There are in fact two types of strings with different boundary conditions, open strings and closed strings:

- *Open strings*

  For the open string we can set $\sigma_0 = l$ ans thus $\sigma \in (0, l)$. These type of strings satisfy either NEUMANN boundary conditions

$$\partial_\sigma X^M(\tau,\sigma)\big|_{\sigma=0,l} = 0 \tag{1.1.10}$$

  or DIRICHLET boundary conditions

$$\delta X^M(\tau,\sigma)\big|_{\sigma=0,l} = 0. \tag{1.1.11}$$

- *Closed strings*

  Here we usually set $\sigma_0 = 2\pi$ leading to $\sigma \in [0, 2\pi)$. This type of string satisfies periodic boundary conditions

$$\begin{aligned} X^M(\tau,0) = X^M(\tau,2\pi), \qquad \partial_\sigma X^M(\tau,\sigma)\big|_{\sigma=0} = \partial_\sigma X^M(\tau,\sigma)\big|_{\sigma=2\pi}, \\ h_{\alpha\beta}(\tau,0) = h_{\alpha\beta}(\tau,2\pi). \end{aligned} \tag{1.1.12}$$

One can then exploit the symmetries of the POLYAKOV action to give the string equations of motion a rather simple form. For instance, one can use the local symmetries to choose a convenient gauge in which the worldsheet metric is conformally flat

$$h_{\alpha\beta} = \Omega^2(\sigma)\eta_{\alpha\beta}, \quad \text{with} \quad \eta_{\alpha\beta} = \mathrm{diag}(-,+). \tag{1.1.13}$$

In this conformal gauge the POLYAKOV action takes the form

$$S_{\mathrm{P}} = \frac{1}{4\pi\alpha'} \int \mathrm{d}^2\sigma \, \left(\partial_\tau X^M \partial_\tau X^N - \partial_\sigma X^M \partial_\sigma X^N\right) \eta_{MN} \tag{1.1.14}$$

which is leading to the simple equations of motion

$$\left(\partial_\tau^2 - \partial_\sigma^2\right) X^M = 0. \tag{1.1.15}$$

Their solutions are well known and can be derived by decomposition into FOURIER modes.

1.2 Superstring theory

The theory considered so far describes only bosons and also gives rise to unphysical tachyon states. To apply string theory to naturally observed object it also lacks in the appearance of fermionic degrees of freedom. Those can be included by the introduction of supersymmetry. The supersymmetrized POLYAKOV action also contains the superpartners Ψ^M next to the coordinate fields X^M. In conformal gauge this action reads

$$S_{\mathrm{P}} = -\frac{1}{4\pi\alpha'} \int \mathrm{d}^2\sigma \eta^{\alpha\beta} \left(\partial_\alpha X^M \partial_\beta X^N + i\,\bar{\Psi}\gamma_\alpha\partial_\beta\,\Psi\right) \eta_{MN}. \tag{1.2.1}$$

Here γ_α are 2d DIRAC matrices and Ψ^M can be chosen to be MAJORANA-WEYL spinors $\Psi^M = (\psi_-^M, \psi_+^M)^{\mathrm{T}}$. From the action (1.2.1) one can then derive the DIRAC equation which reduces to two sets of WEYL equations that are given in light-cone coordinates $\sigma_\pm = \tau \pm \sigma$ by

$$\partial_+ \psi_-^M = \partial_- \psi_+^M = 0. \tag{1.2.2}$$

By partial integration of the fermionic part of the action one can find a surface term which imposes boundary conditions. There are again two types:

- *Open strings*

$$\psi_-^M(\tau, 0) = \psi_+^M(\tau, 0), \quad \psi_-^M(\tau, l) = e^{2\pi i\nu}\psi_+^M(\tau, l), \quad \nu = 0, 1/2. \tag{1.2.3}$$

  The corresponding sectors for the values $\nu = 0$ and $\nu = 1/2$ are called RAMOND (R) and NEVEU-SCHWARZ (NS) sectors, respectively.

- *Closed strings*
  For closed strings there are four sectors of the corresponding combinations of periodic (R) or anti-periodic boundary conditions given by

$$\begin{aligned} \psi_-^M(\tau, \sigma + 2\pi) &= e^{2\pi i\nu}\psi_-^M(\tau, \sigma) \\ \psi_+^M(\tau, \sigma + 2\pi) &= e^{2\pi i\nu'}\psi_+^M(\tau, \sigma). \end{aligned} \tag{1.2.4}$$

With help of a so called GSO projection it is possible to project out all tachyon states and leave an equal number of bosons and fermions at each mass level. This helps to give rise to supersymmetry also in target space.

1.3 Strings in curved backgrounds

For now we have only considered strings propagating in flat MINKOWSKI target space. To impose a more general application to string theory, one also has to take other backgrounds into account. Therefore we promote the target space metric $\eta_{MN} \to g_{MN}(X)$, leading to the bosonic POLYAKOV action

$$S_{\mathrm{P}} = -\frac{1}{4\pi\alpha'} \int_\Sigma \mathrm{d}^2\sigma \sqrt{-h} h^{\alpha\beta} g_{MN}(X) \partial_\alpha X^M \partial_\beta X^N. \tag{1.3.1}$$

This is called the *bosonic non-linear string sigma model*. For the inclusion of supersymmetry this process is not so straight forward any more. Next to the flat ten-dimensional MINKOWSKI space, type IIB supergravity admits $AdS_5 \times S^5$ as another maximally supersymmetric solution as a background (see e.g. [4]) which we are explicitly interested in. This solution is supported by a self-dual RAMOND-RAMOND five-form flux. The difficulties emerging here are due to the non-locality of the RR flux and that it is unclear how to couple it to the string worldsheet. Remarkably this problem has been solved

by Metsaev and Tseytlin in [5] with a GREEN-SCHWARZ type of approach, but unfortunately we will not be able to present the full procedure here due to its complexity and requirement of sophisticated analytical tools. We therefore refer the reader to the original publication. What we will have to deal with in the following is a special solution to to a gauge fixed version of this $AdS_5 \times S^5$ string developed in [5]. But before we come to that, we want to give a brief introduction on how to discretize string theory in order to conduct a numerical study on AdS/CFT from a stringy point of view.

2 Lattice Basics

In this section we want to present the basic concepts of lattice field theory, which has developed to a highly sophisticated research area in the last decades especially in the regime of QCD. This approach to field theory is not only of major concern for performing numerical calculations. It even provides a natural attempt to regularization, which makes it also an interesting topic for theorists in the field of gauge theories.

2.1 Discretizing the worldsheet

A computer is not able to deal with continuous variables, since already a continuous real interval can contain an infinite amount of points, but a computer only has limited memory. Hence we need to limit the amount of points that we consider to make calculations. Since all the target space coordinates[1] depend on the worldsheet coordinates τ and σ, it seems natural to discretize the worldsheet map. We therefore introduce a lattice spacing a and the lattice size in spacial direction L and in time direction T. Following the remarks in [6] we define the two-dimensional lattice Λ to be

$$\Lambda = \{(n_0, n_1) \,|n_0 = 0, 1, \ldots, (T-1)\ ;\ n_1 = 0, 1, \ldots, (L-1)\}\,. \tag{2.1.1}$$

With that we can express the worldsheet coordinates with the lattice coordinates

$$(\tau, \sigma) = (an_0, an_1)\,. \tag{2.1.2}$$

And since the lattice spacing is overall constant we can abbreviatly refer to a field Φ in the theory as a function of the lattice variables $\Phi(n_0, n_1)$. We now further want to discretize differential operators and integrals. The differentiation can be discretized in various ways inspired by its mathematical definition via differential quotients. To see additionally which order of error is introduced compared to the exact derivative, we examine the Taylor expansion of a real function $f(x)$ with a small offset ϵ

$$f(x \pm \epsilon) = f(x) \pm \epsilon f'(x) + \frac{\epsilon^2}{2} f''(x) \pm \frac{\epsilon^3}{6} f'''(x) + \ldots. \tag{2.1.3}$$

Now we can define a forward derivative as the finite difference

$$\frac{f(x+\epsilon) - f(x)}{\epsilon} = f'(x) + \mathcal{O}(\epsilon) \tag{2.1.4}$$

[1] which represent the fields in our two-dimensional QFT

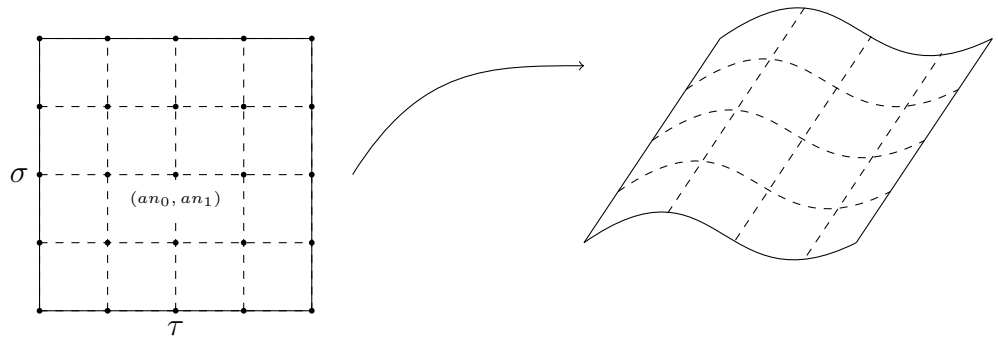

Figure 2.1.1 Mapping of the worldsheet grid into target space.

and in the same way also a backward derivative by using the $f(x-\epsilon)$ term. Combining both leads to the symmetric derivative with an error of higher order in ϵ

$$\frac{f(x-\epsilon)-f(x+\epsilon)}{2\epsilon} = f'(x) + \mathcal{O}(\epsilon^2). \tag{2.1.5}$$

It is more convenient to use the symmetric finite difference, because the error introduced by the finite lattice spacing is hereby reduced by one order. By adding additional terms of $f(x \pm 2\epsilon)$ it is possible to get a finite difference derivative which is exact up to an order of $\mathcal{O}(\epsilon^3)$ and so on. Depending on the demanded accuracy one is able to regulate the introduced error via this method. With ϵ being our lattice spacing a we find the derivative of our fields at $n = (n_0, n_1)$ to be[2]

$$\partial_\alpha \Phi(\tau,\sigma) = \widehat{\partial}_\alpha \Phi(n) + \mathcal{O}(a^2) \equiv \frac{\Phi(n-\hat{\alpha}) - \Phi(n+\hat{\alpha})}{2a} + \mathcal{O}(a^2), \tag{2.1.6}$$

where $\hat{\alpha}$ is the unit vector in α-direction. For the integration over the worldsheet coordinates we replace the integral by a finite sum over all lattice points

$$\int \mathrm{d}\tau \mathrm{d}\sigma \longrightarrow a^2 \sum_{n\in\Lambda}. \tag{2.1.7}$$

For a better visualization it is more convenient to use an abbreviated notation. In the following we will denote $\phi \equiv \phi(n)$ as a field which depends on the lattice coordinates n. The same is true for an operator $M \equiv M(m,n)$. A shorter expression of a matrix-vector like product is given by

$$\phi^T M \psi \equiv \sum_{m,n\in\Lambda} \phi(m) M(m,n) \psi(n)\,. \tag{2.1.8}$$

[2]With $\widehat{\partial}_\alpha$ beeing the symmetric finite difference in α-direction. We also define the forward and backward finite difference respectively by

$$\vec{\partial}_\alpha \Phi(n) = \frac{\Phi(n+\hat{\alpha}) - \Phi(n)}{a} \quad \text{and} \quad \overleftarrow{\partial}_\alpha \Phi(n) = \frac{\Phi(n) - \Phi(n-\hat{\alpha})}{a}.$$

To implement the previous relation on a computer as an actual matrix-vector product it is necessary to map the grid index $n = (n_0, n_1)$ to a lexicographic vector index

$$l(n) = Ln_0 + n_1 \qquad \text{with} \qquad l = 0, 1, \ldots, (V-1), \quad V = LT, \tag{2.1.9}$$

so that the according fields $\phi_{l(n)} \equiv \phi(n)$ are actual vectors and we can apply a matrix-vector notation

$$\phi^{\mathrm{T}} M \phi \equiv \sum_{l,p=0}^{V-1} \phi_l M_{lp} \phi_p, \tag{2.1.10}$$

where then M is also an actual matrix. For the finite differences derivatives we also need to know the neighboring relations. So if we want to move on the grid in direction $\pm\hat{\alpha}$, which lexicographic index corresponds to this movement? These relations are implemented into a *next neighbor* function (nb) which also takes into account the boundary conditions (toroidal in our case) and returns the corresponding vector index

$$l_{\pm\hat{\alpha}} = \mathrm{nb}\,(l, \pm\hat{\alpha}). \tag{2.1.11}$$

We now want to define a symmetric finite difference without the factor $1/a$ for the lexicographic notation by

$$\bar{\Delta}_\alpha \phi_l \equiv \frac{1}{2}\left(\phi_{l_{+\hat{\alpha}}} - \phi_{l_{-\hat{\alpha}}}\right). \tag{2.1.12}$$

In consequence we can write $\bar{\Delta}_\alpha$ as a $V \times V$ matrix

$$\left(\bar{\Delta}_\alpha\right)_{lp} = \frac{\delta_{l_{+\hat{\alpha}},p} - \delta_{l_{-\hat{\alpha}},p}}{2}. \tag{2.1.13}$$

For other than periodic boundary conditions some of the signs have to be flipped according to the relation (D.0.9). In the same way we can define forward and backward finite differences by

$$(\Delta_\alpha)_{lp} = \delta_{l_{+\hat{\alpha}},p} - \delta_{l,p}, \qquad (\Delta^*_\alpha)_{lp} = \delta_{l,p} - \delta_{l_{-\hat{\alpha}},p}. \tag{2.1.14}$$

We will come back to this notation in chapter 4. For now on we will presume using the grid notation for the further studies.

2.2 Bosons and fermions on the lattice

2.2.1 Bosonic propagator

In the examined theory bosons and fermions are both scalar fields of either real, or complex Grassmann type. The equations of motion of bosons are given by the Klein-Gordon equation, which contains only second derivatives. To discretize the second derivative we define the corresponding

finite difference operator simply by applying a forward and a backward finite difference

$$\widehat{\partial}_\alpha^2 \Phi(n) = \overleftarrow{\partial}_\alpha \vec{\partial}_\alpha \Phi(n) = \frac{\Phi(n+\hat{\alpha}) - 2\Phi(n) + \Phi(n-\hat{\alpha})}{a^2}. \tag{2.2.1}$$

In a Lagrangian we would find the differential operator enclosed by the fields, for instance like

$$\Phi(n)\big(\widehat{\partial}_\alpha^2 \Phi\big)(n) = \sum_{m\in\Lambda} \Phi(n)\widehat{\partial}_\alpha^2(n,m)\,\Phi(m), \tag{2.2.2}$$

where we use (2.2.1) to define

$$\widehat{\partial}_\alpha^2(n,m) \equiv \frac{\delta_{m,n+\hat{\alpha}} - 2\delta_{m,n} + \delta_{m,n-\hat{\alpha}}}{a^2}. \tag{2.2.3}$$

To investigate the behaviour of bosons under the discretization we are interested in the propagator, which is the inverse of the differential operator in momentum space. We therefore perform a discrete Fourier transform, which is discussed in Appendix D. Both indices m and n transform independently and in order to perform a unitary similarity transformation the second index is Fourier transformed using the complex conjugated phase [6]

$$\begin{aligned}
\widetilde{\partial}_\alpha^2(p,q) &= \frac{1}{|\Lambda|}\sum_{m,n\in\Lambda} \mathrm{e}^{-iq\cdot na}\,\widehat{\partial}_\alpha^2(n,m)\,\mathrm{e}^{ip\cdot ma} \\
&= \frac{1}{|\Lambda|}\sum_{n\in\Lambda} \mathrm{e}^{-i(q-p)\cdot na}\frac{1}{a^2}\left[\mathrm{e}^{ip_\alpha a} - 2 + \mathrm{e}^{-ip_\alpha a}\right] \\
&= \delta(p-q)\,\widetilde{\partial}_\alpha^2(p),
\end{aligned} \tag{2.2.4}$$

where the Fourier transform of the second derivative is defined by

$$\widetilde{\partial}_\alpha^2(p) \equiv -\frac{4}{a^2}\sin^2\left(\frac{p_\alpha a}{2}\right). \tag{2.2.5}$$

The Euclidean Klein-Gordon operator $\widetilde{D}(p)$ in momentum space with particle mass m reads

$$\widetilde{D}(p) = m^2 + \sum_{\alpha=0}^{1} \widetilde{\partial}_\alpha^2(p). \tag{2.2.6}$$

And so we find the propagator simply by inverting the previous relation. Of special interest is the massless case, where we want to investigate the continuum limit

$$\widetilde{D}^{-1}(p)\Big|_{m=0} = \frac{1}{-\frac{4}{a^2}\sum\limits_{\alpha=0}^{1}\sin^2\left(\frac{p_\alpha a}{2}\right)} \xrightarrow{a\to 0} -\frac{1}{p^2}. \tag{2.2.7}$$

This is precisely what we expected for the Euclidean propagator in the continuum. Since we have $p_\alpha \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$, there are no additional poles within the sine function other than the physical one at $p = (0,0)$.

2.2.2 Fermionic propagator and the doubling problem

In the case of fermions the equations of motion in 4-dimensional QFT are given by the Dirac equation, which is a linearisation of the Klein-Gordon equation and only contains first derivatives. To not explicitly break existing symmetries, we have to go with the symmetric derivative in this case. Now we can follow the exact same steps as for the bosonic case to investigate the continuum limit of a Dirac like operator in our 2-dimensional space time. As mentioned we start from the symmetric finite difference

$$\widehat{\partial}_\alpha(m,n) \equiv \frac{\delta_{m,n+\hat{\alpha}} - \delta_{m,n-\hat{\alpha}}}{2a} \tag{2.2.8}$$

and proceed with the Fourier transform

$$\widetilde{\partial}_\alpha(p,q) = \frac{1}{|\Lambda|} \sum_{m,n\in\Lambda} \mathrm{e}^{-iq\cdot na}\, \widehat{\partial}_\alpha(n,m)\, \mathrm{e}^{ip\cdot ma} \tag{2.2.9}$$

$$= \frac{1}{|\Lambda|} \sum_{n\in\Lambda} \mathrm{e}^{-i(q-p)\cdot na} \left[\frac{\mathrm{e}^{ip_\alpha a} - \mathrm{e}^{-ip_\alpha a}}{2a}\right] \tag{2.2.10}$$

$$= \delta(p-q)\, \widetilde{\partial}_\alpha(p), \tag{2.2.11}$$

here we are left with the following differential operator in momentum space

$$\widetilde{\partial}_\alpha(p) \equiv \frac{i}{a} \sin(p_\alpha a). \tag{2.2.12}$$

To construct an Euclidean Dirac like operator in two dimensions we use the first two Pauli matrices[3]

$$\widetilde{D}_D(p) = m\mathbb{1} + \sum_{\alpha=0}^{1} \gamma_\alpha\, \widetilde{\partial}_\alpha(p) = m\mathbb{1} + \frac{i}{a} \sum_{\alpha=0}^{1} \gamma_\alpha \sin(p_\alpha a)\,. \tag{2.2.13}$$

The inverse propagator follows from the properties of the Pauli matrices to be

$$\widetilde{D}_D^{-1}(p) = \frac{m\mathbb{1} - \frac{i}{a}\sum_{\alpha=0}^{1} \gamma_\alpha \sin(p_\alpha a)}{m^2 + a^{-2}\sum_{\alpha=0}^{1} \sin^2(p_\alpha a)}. \tag{2.2.14}$$

Once more we want to study the continuum limit of the propagator for the massless case and find by setting $m = 0$

$$\widetilde{D}_D^{-1}(p)\Big|_{m=0} = \frac{-\frac{i}{a}\sum_{\alpha=0}^{1} \gamma_\alpha \sin(p_\alpha a)}{a^{-2}\sum_{\alpha=0}^{1} \sin^2(p_\alpha a)} \xrightarrow{a\to 0} \frac{-i\sum_{\alpha=0}^{1} \gamma_\alpha p_\alpha}{p^2}. \tag{2.2.15}$$

Here again the propagator has the correct naive continuum limit but this time we face another problem. Since again p_α is in the domain $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$,

[3]
$$\gamma_0 = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \gamma_1 = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

there occur three other non-physical poles within the sine function at $p = (0, \pi/a)$, $p = (\pi/a, 0)$ and $p = (\pi/a, \pi/a)$. As a result in the numerical simulation it seems that there are in this case three additional fermions, which emerge only from the method of discretization and are non-physical. This is obviously leading to distorted calculations and needs to be circumvented. That particular problem is known as fermion doubling and has been investigated extensively by WILSON, who introduced a possible solution. He suggested to add a term proportional to the discretized LAPLACE operator[7], which is known as a WILSON term. We can express it in momentum space with the help of (2.2.5) and find[4]

$$W(p) \equiv -\mathbb{1}\frac{a}{2}\sum_{\alpha=0}^{1}\widetilde{\partial}_{\alpha}^{2}(p) = \mathbb{1}\frac{1}{a}\sum_{\alpha=0}^{1}\left(1-\cos(p_\alpha a)\right). \tag{2.2.16}$$

Since the LAPLACE operator is of order $\mathcal{O}(a^0)$, we see that the WILSON term vanishes in the continuum limit. It also vanishes for $p_\alpha = 0$ and therefore gives no contribution to the physical pole of the theory. If we now invert the new DIRAC-WILSON operator

$$\widetilde{D}_W(p) \equiv \widetilde{D}_D(p) + W(p), \tag{2.2.17}$$

we find the new massless momentum space propagator

$$\widetilde{D}_W^{-1}\Big|_{m=0} = \frac{\mathbb{1}\frac{1}{a}\sum_{\alpha=0}^{1}\left(1-\cos(p_\alpha a)\right) - \frac{i}{a}\sum_{\alpha=0}^{1}\gamma_\alpha \sin(p_\alpha a)}{\left(\frac{1}{a}\sum_{\alpha=0}^{1}\left(1-\cos(p_\alpha a)\right)\right)^2 + \frac{1}{a^2}\sum_{\alpha=0}^{1}\sin^2(p_\alpha a)}. \tag{2.2.18}$$

Here we can convince ourselves, that there are no more additional poles in the domain of p_α, since for the points where $p_\alpha = \pi/a$ the denominator does not vanish like before. Actually for these points the WILSON-term behaves like an additional mass term that is growing infinitely in the continuum limit and consequently decouples from the theory.

2.3 Monte Carlo methods

Now after we know, how to discretize differential operators and act with them on bosonic and fermionic quantities, we are able to build a discretized Lagrangian as well. But what we really need is a method to perform the calculation of observables in the path integral formalism. In QFT in the continuum we calculate the expectation value of an observable O via [8]

$$\langle O \rangle = \frac{1}{Z}\int \mathcal{D}\phi\, O(\phi)\exp\left(-S\left[\phi\right]\right), \tag{2.3.1}$$

[4] using the identity

$$\begin{aligned} & \cos(2x) = \cos^2(x) - \sin^2(x) \\ \Leftrightarrow \quad & \sin^2(x) = \tfrac{1}{2}\left(1-\cos(2x)\right) \end{aligned}$$

where S is the EUCLIDEAN action depending on the collection of fields ϕ and Z is the partition function

$$Z = \int \mathcal{D}\phi \, \exp\left(-S\left[\phi\right]\right). \tag{2.3.2}$$

In fact there is no rigorous mathematical definition for the path integral in the continuum. It is motivated from a discretized measure, which is then somehow said to be made continuus. This step is considered ill defined by most mathematicians, but since we stay on a discretized lattice, the path integral measure $\mathcal{D}\phi$ can be perfectly well defined and is represented by

$$\mathcal{D}\phi = \prod_{n\in\Lambda} \mathrm{d}\phi(n). \tag{2.3.3}$$

This means, that for every lattice point a multidimensional integral needs to be calculated. Even for small lattices this task becomes tortuous and soon even supercomputers would not be able to do that calculation in reasonable time. Out of this reason other methods of calculation have been considered. The most favoured one is a statistical method going under the name of Monte Carlo simulation. With this type of calculation it is possible to obtain good statistical approximations of high-dimensional integrals in reasonable time. At this point we want to study some details of the Monte Carlo methods used in the scope of this thesis.

2.3.1 Monte Carlo integration

The easiest way to understand the idea behind any form of calculation with Monte Carlo methods is via the Monte Carlo integration. Suppose we want to calculate the following multi-dimensional integral

$$I = \int_\Omega f(x)\,\mathrm{d}x, \tag{2.3.4}$$

where $\Omega \subset \mathbb{R}^n$ is a compact integration domain. Then probability theory tells us [9], that we can approximate the integral I with a set of random numbers $\{\overline{x}_1, \ldots, \overline{x}_N\}$ uniformly distributed on Ω with

$$I_N = V\frac{1}{N}\sum_{i=1}^{N} f(\overline{x}_i). \tag{2.3.5}$$

Hereby $V = \int_\Omega \mathrm{d}x$ denotes the integration volume. One can show that I_N approximates I up to an error of order $\mathcal{O}(1/\sqrt{N})$ and the law of large numbers tells us, that $\lim\limits_{N\to\infty} I_N = I$. One can also write for the expectation value $\langle f\rangle$ of f, that

$$\langle f\rangle = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N} f(\overline{x}_i) = \frac{\int_\Omega f(x)\,\mathrm{d}x}{\int_\Omega \mathrm{d}x}. \tag{2.3.6}$$

An instructive example is to calculate the value of π with the 2D-integral $I = \int_\Omega H(x,y)\,\mathrm{d}x\mathrm{d}y$ over the domain $\Omega = [-1,1]\times[-1,1]$ with the function

$$H(x,y) = \begin{cases} 1 & \text{if} \quad x^2+y^2 \leq 1 \\ 0 & \text{else.} \end{cases} \tag{2.3.7}$$

Analytically we know that I corresponds to the area of the unit circle and has the value $I = \pi$. With the volume being $V = 4$ we can find an estimate

$$\pi \approx \frac{4}{N}\sum_{i=1}^{N} H(\overline{x}_i). \tag{2.3.8}$$

This means that we can estimate the value of $\pi/4$ by counting the number of points lying within the circle (see figure 2.3.1) and dividing by the total number of points.

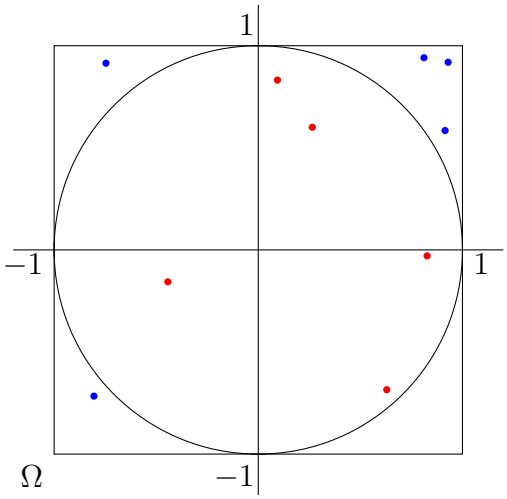

Figure 2.3.1 Graphic of random numbers uniform in Ω. $\pi/4$ can be estimated by the number of red points within the circle divided by total number of points.

2.3.2 Importance sampling and Markov chains

More generally one can estimate integrals over a function $f(x)$ multiplied with a certain weight function $\rho(x)$ in the same way. We can write for the expectation value

$$\langle f\rangle_\rho \equiv \frac{\int_\Omega f(x)\rho(x)\,\mathrm{d}x}{\int_\Omega \rho(x)\,\mathrm{d}x} = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N} f(\overline{x}_i). \tag{2.3.9}$$

But in this case the random numbers $\overline{x}_i$ need to be distributed through the weight function $\rho(x)$. For this to be possible $\rho(x)$ needs to be a valid probability density function. Comparing with (2.3.1) we can convince ourselves, that this is the case for the EUCLIDEAN path integral. We can exploit

this fact to make our calculation more efficient. In principle one could go with the simple Monte Carlo integration scheme, but since our integration domain is no compact interval but the $\mathbb{R}^n$, we would produce lots of configurations that would give no contribution to the path integral due to the weight factor and therefore introduce a large error. So if we produce random configurations distributed through a probability density given by the weight factor, we would generate mostly configurations with a non vanishing contribution and the statistical error will be reduced. This procedure is called importance sampling. But to do the importance sampling one needs to be able to produce random configurations according to the given probability density. Since the action appearing in this probability density is in general a very complicated function, this task becomes highly non trivial and there usually is no way to directly transform uniformly distributed random configurations into the favoured form. To make this more explicit, consider the one dimensional integral with normalized probability density function [10]

$$\langle f \rangle_\rho = \int_a^b f(x)\rho(x)\,\mathrm{d}x\,, \quad \int_a^b \rho(x)\,\mathrm{d}x = 1. \tag{2.3.10}$$

The distribution function $P(x)$ is given by

$$P(x) = \int_a^x \rho(t)\,\mathrm{d}t. \tag{2.3.11}$$

If we perform the substitution

$$y(x) \equiv P(x), \quad \text{with} \quad \rho(x) = P'(x) = y'(x), \quad y \in [0,1], \tag{2.3.12}$$

we are left with

$$\langle f \rangle_\rho = \int_a^b f(x)y'(x)\,\mathrm{d}x = \int_0^1 f\left(x\left(y\right)\right)\mathrm{d}y, \tag{2.3.13}$$

where $x(y) = P^{-1}(y)$. So if we generate uniformly distributed random numbers $\overline{y}$ and use $\overline{x} = P^{-1}(\overline{y})$, which is now distributed according to $\rho(x)$, we can write

$$\langle f \rangle_\rho = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(\overline{x}_i). \tag{2.3.14}$$

For this to be true $P(x)$ needs to be strongly increasing and globally invertible. Extended to the higher-dimensional problem of path integrals this demand is met very unlikely, as said before.

To circumvent this issue one uses a statistical model called Markov chain to obtain configurations that are distributed according to the Boltzmann factor of the path integral. The idea is to start from an arbitrary configuration and generate a new one from the previous configuration via

a pseudo random number generation process. Thereby new configurations are generated in a stochastic sequence that eventually follows an equilibrium distribution $P(\phi)$ [6]. The configurations in the chain can be numbered by an index, the so called Monte Carlo time

$$\phi_0 \to \phi_1 \to \ldots \to \phi_{N_{\text{th}}} \to \ldots \,. \tag{2.3.15}$$

The first configurations up to an index N_{th} should not be used for measurements since they are most certainly not properly distributed. The process needs a specific amount of time to reach its equilibrium distribution. Therefore this period is called equilibration or thermalization phase. A Markov process is characterized by a conditional transition probability $T(\phi'|\phi)$ to move from a configuration ϕ to ϕ'. This probability depends only on the configurations ϕ and ϕ' and not any previous ones. It obeys the properties

$$0 \leq T(\phi'|\phi) \leq 1, \quad \sum_{\phi} T(\phi'|\phi) = 1. \tag{2.3.16}$$

An important restriction is that the process must not get stuck at any configuration. It must always be possible to move between two specified configurations within a finite Monte Carlo time. This can be realised if the transition probability is strictly positive between all states which is called strong ergodicity. Furthermore the probability to move to ϕ' from any other state must be the same as to leave ϕ' to any other state which can be condensed to the following balance equation

$$\sum_{\phi} T(\phi'|\phi)P(\phi) = \sum_{\phi} T(\phi|\phi')P(\phi'). \tag{2.3.17}$$

A special solution to this equation will be obtained if one assumes that the equation holds for every term of the sum

$$T(\phi'|\phi)P(\phi) = T(\phi|\phi')P(\phi'). \tag{2.3.18}$$

This condition is called detailed balance and is used by most algorithms generating Markov chains.

2.3.3 Fermions on the lattice and the hybrid Monte Carlo algorithm

There are many possible algorithms to generate field configurations. The choice is depending on the structure of the problem at hand. For the here presented case the algorithm of choice is called rational hybrid Monte Carlo (RHCM). The basic reason to use this algorithm is the presence of fermions in a specific manner. It is in general complicated to deal with fermions in numerical simulations due to the anti commuting properties of Grassmann variables. An efficient procedure is to integrate out fermions via Grassmann integration, presented in Appendix A.2, which results in our case in

the PFAFFIAN of a fermionic operator $M[\phi]$ depending on the bosonic fields ϕ. We now want to include the PFAFFIAN as a probability weight factor in the process of generating MARKOV chain configurations. To act as a probability weight factor, $\mathrm{Pf}\, M$ must be real and nonnegative. If we consider this to be the case for the moment, we can write

$$\mathrm{Pf}\, M = (\det M)^{\frac{1}{2}} = \left(\det MM^\dagger\right)^{\frac{1}{4}}. \tag{2.3.19}$$

In general one could have to deal with an arbitrary fraction α in the exponent on the right side of (2.3.19). If we restrict $\mathrm{Pf}\, M$ to be also nonzero and therefore entirely positive using that $MM^\dagger$ is positive definite, one can rewrite the determinant as a bosonic path integral with pseudofermions ξ

$$\left(\det MM^\dagger\right)^\alpha = \frac{1}{\det\left(MM^\dagger\right)^{-\alpha}} \sim \int \mathcal{D}\eta\, \mathcal{D}\eta^\dagger\; e^{-\xi^\dagger (MM^\dagger)^{-\alpha}\xi}. \tag{2.3.20}$$

Since there is an inversion included, the operator in the exponent is highly nonlocal in the bosonic fields ϕ. So even a small change in the fields could cause a large difference in the weight factor. Ergo one needs an algorithm that ensures that the generated configurations are part of the contributing regime of the weight factor. In a case like that it proved efficient to use a hybrid Monte Carlo (HMC) algorithm when $\alpha = 1$, which uses HAMILTONIAN dynamics trajectories along some fictitious time to generate new configurations. For non-integer α one can use a rational approximation of $\left(MM^\dagger\right)^{-\alpha}$. Combined with the HMC this is called the rational hybrid Monte Carlo (RHMC) algorithm.

At this point we want to introduce the HMC algorithm which has been proposed in [11]. A more detailed explanation is presented in [6, 7] which serves as a guideline for the following. The HMC is referred to as hybrid because it combines a molecular dynamic (MD) evolution with random noise patterns to simulate quantum fluctuations, an additional METROPOLIS acceptance step lets it result into an exact MC algorithm. The field update is separated into two phases. Pseudofermions are updated first with an exact heat bath, while the bosons are kept constant. Therefore, a configuration ϑ is generated from a GAUSSIAN distribution $P(\vartheta) \sim e^{-\vartheta^\dagger\vartheta}$ and we set $\xi = M\vartheta$. In the second phase a molecular dynamic evolution is used to update the bosonic fields while the pseudofermions are kept constant. We can now think of the effective action $S_{\mathrm{eff}}[\phi] = S_{\mathrm{B}}[\phi] + \xi^\dagger (MM^\dagger)^{-1}\xi$ as only dependent on the bosonic fields ϕ. Now for each field ϕ_i a conjugate momentum π_i is introduced and we expand the path integral with $\int \mathcal{D}\pi\, \exp(-1/2\, \pi^2)$ to obtain

$$\langle O\rangle = \frac{\int \mathcal{D}\phi\mathcal{D}\eta\mathcal{D}\pi\; O(\phi)\, e^{-H[\phi,\pi]}}{\int \mathcal{D}\phi\mathcal{D}\eta\mathcal{D}\pi\; e^{-H[\phi,\pi]}}, \tag{2.3.21}$$

where we have introduced the HAMILTONIAN

$$H[\phi,\pi] = \frac{1}{2}\pi^2 + S_{\mathrm{eff}}[\phi]\,, \quad \pi^2 = \sum_i \sum_{n\in\Lambda} \pi_i^2(n)\,. \tag{2.3.22}$$

The evolution of the fields follows according to the classical equations of motion along a fictitious MC time τ

$$\begin{aligned}\dot{\pi}_i &= -\frac{\partial H}{\partial \phi_i} = -\frac{\partial S_{\text{eff}}}{\partial \phi_i} \\ \dot{\phi}_i &= \frac{\partial H}{\partial \pi_i} = \pi_i\end{aligned} \tag{2.3.23}$$

A numerical implementation of (2.3.23) introduces a discrete step size $\epsilon \equiv \delta\tau$ and errors of order $\mathcal{O}(\epsilon^2)$. An additional Metropolis acceptance step can correct these errors. First the momenta π are randomly generated from a Gaussian distribution $P_{\text{G}}(\pi) = \exp(-1/2\,\pi^2)$. Then a numerical integration scheme is used to change the configuration $\{\phi, \pi\}$ along a discretized trajectory in phase space to the new point $\{\phi', \pi'\}$. The transition probability $T_{\text{MD}}(\phi', \pi'|\phi, \pi)$ of the MD evolution depends on the integration scheme. The latter needs to be reversible and area preserving for the algorithm to obey detailed balance. Thus, a *leapfrog integration* scheme is used. For one trajectory the fields ϕ are evolved in n steps of length ϵ. The momenta start with half a step of length $\epsilon/2$, then $(n-1)$ full steps are performed and again a half-step. The first half-step is given by

$$\begin{aligned}\pi_i(\tfrac{\epsilon}{2}) &= \pi_i(0) - \frac{\partial S_{\text{eff}}(\phi(0))}{\partial \phi_i}\frac{\epsilon}{2}, \\ \phi_i(\epsilon) &= \phi_i(0) + \pi_i(\tfrac{\epsilon}{2})\epsilon\,.\end{aligned} \tag{2.3.24}$$

The next steps for $j = 1, \ldots, n-1$ are

$$\begin{aligned}\pi_i\left(\left(j+\tfrac{1}{2}\right)\epsilon\right) &= \pi_i\left(\left(j-\tfrac{1}{2}\right)\epsilon\right) - \frac{\partial S_{\text{eff}}(\phi(j\epsilon))}{\partial \phi_i}\epsilon \\ \phi_i\left((j+1)\,\epsilon\right) &= \phi^i\left(j\epsilon\right) + \pi_i\left(\left(j+\tfrac{1}{2}\right)\epsilon\right)\epsilon\,.\end{aligned} \tag{2.3.25}$$

With the last half-step we arrive at the final momentum

$$\pi_i(n\epsilon) = \pi_i\left(\left(n+\tfrac{1}{2}\right)\epsilon\right) - \frac{\partial S_{\text{eff}}(\phi(n\epsilon))}{\partial \phi_i}\frac{\epsilon}{2}\,. \tag{2.3.26}$$

With an additional Metropolis acceptance step

$$T_{\text{A}}(\phi', \pi'|\phi, \pi) = \min(1, \exp(H[\phi, \pi] - H[\phi', \pi']) \tag{2.3.27}$$

the total transition probability to move from ϕ to ϕ' is given by

$$T(\phi'|\phi) = \int \mathcal{D}\pi' \mathcal{D}\pi\; T_{\text{A}}(\phi', \pi'|\phi, \pi) T_{\text{MD}}(\phi', \pi'|\phi, \pi) P_{\text{G}}(\pi)\,. \tag{2.3.28}$$

This has been proved to obey detailed balance in [11]. Concluding one can summarize the HMC algorithm in the following steps:

- **Pseudofermions**
  Generate the pseudofermion field $\xi = M\vartheta$, where ϑ is distributed according to $\exp(-\vartheta^\dagger\vartheta)$.

- **Conjugate fields**
  For an initial boson configuration $\phi^{(0)}$ generate $\pi^{(0)}$ according to the GAUSSIAN distribution $\exp(-\frac{1}{2}\pi^2)$.

- **Initial step**
  $\pi_i^{(\frac{1}{2})} = \pi_i^{(0)} - \frac{\epsilon}{2} F_i\left[\phi\right]\Big|_{\phi^{(0)}}$.

- **Intermediate steps**
  Full steps for $j = 1, \ldots, n-1$
  $\phi_i^{(j)} = \phi_i^{(j-1)} + \pi_i^{(j-\frac{1}{2})}$, $\qquad \pi_i^{(j+\frac{1}{2})} = \pi_i^{(j-\frac{1}{2})} - \epsilon F_i\left[\phi\right]\Big|_{\phi^{(j)}}$.

- **Final step**
  $\phi_i' = \phi_i^{(n)} = \phi_i^{(n-1)} + \pi_i^{(n-\frac{1}{2})}$, $\quad \pi_i' = \pi_i^{(n)} = \pi_i^{(n-\frac{1}{2})} - \frac{\epsilon}{2} F_i\left[\phi\right]\Big|_{\phi^{(n)}}$.

- **Monte Carlo step**
  Accept new configuration ϕ' if a random number $r \in [0,1)$ is smaller than

$$\exp\left(\frac{1}{2}\left(\pi^2 - \pi'^2\right) + S_{\mathrm{B}}[\phi] - S_{\mathrm{B}}[\phi'] + \vartheta^\dagger\vartheta - \xi^\dagger\left(M'M'^\dagger\right)^{-1}\xi\right).$$

Here we used $\phi_i^{(j)} \equiv \phi_i(j\epsilon)$ and the driving forces are denoted by

$$F_i[\phi] = \frac{\partial}{\partial\phi_i}\left[S_{\mathrm{B}}\left[\phi\right] + \xi^\dagger\left(MM^\dagger\right)^{-1}\xi\right]. \tag{2.3.29}$$

2.3.4 The numerical sign problem

As discussed previously we want to calculate expectation values of observables $O(\phi)$, depending on bosonic fields ϕ which are distributed according to a certain probability weight function $\rho(\phi)$

$$\langle O\rangle_\rho = \frac{\int \mathcal{D}\phi\; O(\phi)\rho(\phi)}{\int \mathcal{D}\phi\; \rho(\phi)}. \tag{2.3.30}$$

The feasibility of calculations like that via Monte Carlo methods is only guaranteed if the weight function $\rho(\phi)$ is non-negative. In the process of dealing with fermions it is sometimes necessary to introduce bosonic auxiliary fields by a HUBBARD-STRATONOVICH (HS) transformation[5] which might lead to a complex phase in the weight function. For fluctuations of this phase that are very close to the purely real spectrum, this can be corrected by a reweighting procedure. If nonetheless the phase is distributed on the whole complex spectrum where the reweighting tends to fail, then one is talking of a *sign problem*. There are several approaches to fix this issue but none of them works as a general method to cure the sign problem.

[5] See Appendix A.3 for futher details on the HS transformation.

3 Preliminaries

3.1 AdS/CFT correspondence

Among the most exciting breakthroughs in theoretical physics in the last decades there certainly is the famous conjecture made by Maldacena in 1997 [12], now widely known as AdS/CFT correspondence which attracted many scientists to contribute their work to this field of study.
What makes this conjecture so promising is that it relates a quantum field theory (QFT) of gauge fields in flat spacetime with a string theory. The latter one is also a promising candidate for a theory of quantum gravity. Unifying gravity with the other fundamental forces condensed in the Standard Model would be one of the next big milestones in physics. By studying the predictions of the AdS/CFT correspondence scientists hope to get one step closer to this fundamental aim. The conjecture links two theories, very different in their physical content and interpretation, stating that they are mathematically equivalent. The AdS part refers to a gravity theory on asymptotically Anti-de Sitter spacetime, CFT stands for conformal field theory. In its primary form [3], the correspondence states that

Type IIB superstring theory
with string length $l_\mathrm{s} = \sqrt{\alpha'}$ and coupling constant g_s on $AdS_5 \times S^5$
with radius of curvature R and N units of $F_{(5)}$ flux on S^5

$\uparrow$ *is dynamically equivalent to* $\downarrow$

$\mathcal{N} = 4$ Super Yang-Mills theory
with gauge group $SU(N)$ and Yang-Mills coupling constant g_YM.

By the conjecture the free parameters on the field theory side g_YM and N are mapped to the free parameters g_s and $R/\sqrt{\alpha'}$ on the string theory side by

$$\frac{4\pi\lambda}{N} = g_\mathrm{s} \quad \text{and} \quad \lambda \equiv g_\mathrm{YM}^2 N = \frac{R^4}{\alpha'^2}\,. \tag{3.1.1}$$

In the second equation we defined the 't Hooft coupling λ. String theory is yet best understood in the perturbative regime, therefore it is convenient to restrict the coupling on the string theory side to $g_s \ll 1$, while keeping $R/\sqrt{\alpha'}$ constant. The AdS side reduces then, at leading order in g_s to classical string theory. The quantity R^2/α' is kept constant. Also the coupling on the CFT side is conveniently taken to be small, $g_{YM} \ll 1$, while $g_{YM}^2 N$ is kept finite. We therefore have to take the large N limit $N \to \infty$ with λ fixed, which is also known as the 't Hooft limit. This corresponds to the planar limit of the gauge theory. We are then left with λ as the free parameter of the AdS/CFT system. In the limit of large λ, and therefore $\alpha'/R^2 \to 0$ or large curvature R, the string does not feel the effect of the interaction created by the (now weakly curved) background. So for large λ one is in the perturbative regime of string theory, whereas the gauge theory side is perturbatively accessible for $\lambda \ll 1$. The fact that the perturbative (accessible) regimes of both models do not overlap - which is referred to as a weak-strong coupling duality - is on one side very fascinating, as it allows the exploration of the strong coupling regime of a theory via the study of the much simpler dual model. On the other side, it makes highly non-trivial any dynamical and direct check of the AdS/CFT correspondence. In this thesis we address the problem of realizing such direct checks numerically within the string worldsheet model. In the latter, we control the large λ regime where we know analytical solutions. The lattice, numerical approach will allow us to leave the perturbative regime and go to smaller λ, where comparison with the solutions of perturbative gauge theory is - once the difficulties peculiar to this approach are tamed - possible. In fact, in the case under study we can also attempt a comparison between string and gauge theory at finite values of λ, where together with the AdS/CFT hypothesis another powerful conjecture - the integrability of the underlying system - is available with its predictions.

3.2 Wilson loops

An important class of observables in gauge theories are non-local gauge invariant operators called Wilson loops. These operators are evaluated along a given closed path $\mathcal{C}$. For specific cusped paths one can (in a certain limit) extract a function, called cusp anomaly, from the Wilson loop. According to AdS/CFT the minimal surface of a string ending on a certain path gives (in a certain regime) the value of the corresponding Wilson loop. We therefore can extract information about the cusp anomaly function also from the string theory side. To make this remark more explicit, we first want to review some more details about Wilson loops.
For pure Yang-Mills theory with the gauge group $SU(N)$ the Wilson loop $W[\mathcal{C}]$ is a path-ordered exponential of a gauge field A_μ along a closed

contour $\mathcal{C}$, which in the fundamental representation is defined by

$$W[\mathcal{C}] = \frac{1}{N}\mathrm{Tr}\left(\mathcal{P}\exp\left[i\oint_{\mathcal{C}} \mathrm{d}x^\mu A_\mu\right]\right). \tag{3.2.1}$$

Here the trace is over the fundamental representation of the gauge group and $\mathcal{P}$ is the path ordering operator. If we choose to parametrise the curve $\mathcal{C}$ as $x^\mu(s)$ with $s \in [0,1]$, we can write the exponent as

$$i\oint_{\mathcal{C}} \mathrm{d}x^\mu A_\mu = i\int_0^1 \mathrm{d}s \frac{\mathrm{d}x^\mu}{\mathrm{d}s} A_\mu\left(x\left(s\right)\right). \tag{3.2.2}$$

Actually we have $A_\mu = A_\mu^a T_a$, where T_a is a generator of the Lie algebra $\mathfrak{su}(N)$ of the gauge group and therefore different fields A_μ do not commute in general. To avoid appearing ambiguities in the ordering of fields due to a Taylor expansion of the exponential, the operator $\mathcal{P}$ is ordering them in the following sense

$$\mathcal{P}\left(A\left(x\left(s_1\right)\right)A\left(x\left(s_2\right)\right)\right) = \begin{cases} A\left(x\left(s_1\right)\right)A\left(x\left(s_2\right)\right) & \text{for } s_1 > s_2, \\ A\left(x\left(s_2\right)\right)A\left(x\left(s_1\right)\right) & \text{for } s_2 > s_1. \end{cases} \tag{3.2.3}$$

3.3 Wilson loops in AdS/CFT

Since the action of four-dimensional $\mathcal{N}=4$ SYM can be derived via dimensional reduction from $\mathcal{N}=1$ SYM in ten dimensions [13] one can construct a Wilson loop there, starting from its definition in the ten dimensional gauge theory. By using the field theory content of the four-dimensional theory A_μ and x^μ and six additional scalar fields of $SU(N)$ the so called Maldacena-Wilson loop proposed in [14] can be written as

$$\mathcal{W}[\mathcal{C}] = \frac{1}{N}\mathrm{Tr}\mathcal{P}\exp\left(\int_{\mathcal{C}} \mathrm{d}s\left(iA_\mu(x)\dot{x}^\mu + |\dot{x}|\phi_I(x)n^I\right)\right). \tag{3.3.1}$$

Here $I = 1,\ldots,6$ and n^I might be considered coordinates in S^5, satisfying $\delta_{IK}n^I n^K = 1$. The curve described by $n^I(s)$ in the five-sphere must not necessarily be closed.
In the context of AdS/CFT the Maldacena-Wilson loop also has a corresponding string theory description, which was first proposed in [14]. Thus the expectation value of the Maldacena-Wilson loop operator is given by a string partition function

$$\langle\mathcal{W}[\mathcal{C}]\rangle = Z_{\text{string}}[\mathcal{C}], \tag{3.3.2}$$

which is a path integral obeying suitable boundary conditions

$$Z_{\text{string}}[\mathcal{C}] = \int_{\partial X^\mu = \mathcal{C}} \mathcal{D}X^M\,\mathcal{D}h_{\alpha\beta}\,\exp\left(-S_{\text{string}}\left(X,h\right)\right). \tag{3.3.3}$$

Here S_{string} is the action of the fundamental string in $AdS_5 \times S^5$, $h_{\alpha\beta}$ a 2d metric and $X^M = (X^\mu, X^{3+I})$ $(M = 0, \ldots, 9;\ \mu = 0, \ldots, 3;\ I = 1, \ldots, 6)$ are the embedding functions in the string target space, depending on the worldsheet coordinates $(\tau, \sigma) \in \Sigma$ where Σ representing a map of the string worldsheet. By defining $\widetilde{X}^I = X^{3+I}$ and therefore $X^M = (X^\mu, \widetilde{X}^I)$ the partition function (3.3.3) needs to meet the following boundary conditions

$$X^\mu|_{\partial\Sigma} = x^\mu(s)\,, \quad \left.\frac{\widetilde{X}^I}{|\widetilde{X}^I|}\right|_{\partial\Sigma} = n^I(s)\,, \quad |\widetilde{X}^I|\Big|_{\partial\Sigma} = 0\,, \tag{3.3.4}$$

where $x^\mu(s)$ parametrises the curve $\mathcal{C}$. One can show that the conformal boundary of $AdS_5 \times S^5$ is 4d Minkowski space[1]. Therefore one can say that the embedding of the string worldsheet is bounded by the curve $\mathcal{C}$, see Figure 3.3.1. In the large 't Hooft coupling limit $\lambda \gg 1$, the path integral (3.3.3) can be evaluated with a saddle point approximation and results in the exponential of a minimal surface $\mathcal{A}_{\min}(\mathcal{C})$ bounded by $\mathcal{C}$

$$\langle \mathcal{W}[\mathcal{C}] \rangle \simeq \exp\left(\frac{\sqrt{\lambda}}{4\pi}\mathcal{A}_{\min}(\mathcal{C})\right). \tag{3.3.5}$$

The dimensional scale $\sqrt{\lambda}/4\pi$ is set by the AdS/CFT mapping (3.1.1) which determines $1/\alpha' = \sqrt{\lambda}$ as it is common in the literature (e.g. [15]) to set the AdS radius to $R = 1$. From the pre factor of the action in the non-linear sigma model (1.3.1) we then find

$$\frac{1}{4\pi\alpha'} = \frac{\sqrt{\lambda}}{4\pi}. \tag{3.3.6}$$

In the following we will also make use of a new defined coupling $g \equiv \sqrt{\lambda}/4\pi$.

3.4 The cusp anomalous dimension of $\mathcal{N} = 4$ SYM

To approach a numerical study of AdS/CFT it is important to consider an observable quantity that is widely known in different ranges of the 't Hooft coupling λ, so its study may act as a guideline in discretizing the theory. One such quantity is the cusp anomaly function (or scaling function). It was first studied as the anomalous dimension of twist two operators in $\mathcal{N} \geq 4$ SYM

$$\mathcal{O}_{\{\mu_1 \cdots \mu_S\}} = \operatorname{Tr} \phi \nabla_{\{\mu_1} \cdots \nabla_{\mu_S\}} \phi\,, \tag{3.4.1}$$

where ϕ is a scalar field of SYM and ∇_μ is the covariant derivative with the indices $\{\mu_1 \cdots \mu_S\}$ being symmetrized. The conformal dimension of such

[1] At the conformal boundary the five-sphere appears to have zero extent. See (B.1) for details on the conformal mapping of AdS_5 to flat 4d Minkowski space.

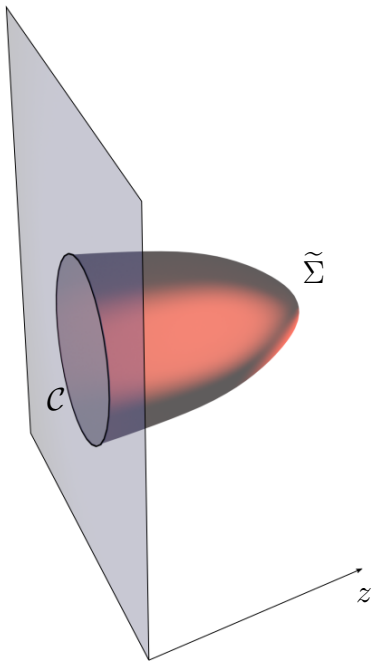

Figure 3.3.1 The embedding of the string worldsheet $\widetilde{\Sigma}$ in $AdS_5 \times S^5$ is bounded by the contour $\mathcal{C}$ as z approaches zero.

operators is $\Delta_S = S + 2 + \gamma_S(\lambda)$ with γ_S being the anomalous dimension and $\gamma_S \sim \ln S$ for $S \to \infty$. In [16] it was proposed that this conformal dimension corresponds to the energy of strings rotating in AdS, that for large S (and in the large λ regime) reads.

$$E \simeq S + \frac{\sqrt{\lambda}}{\pi} \ln S, \quad (S \to \infty)\,. \tag{3.4.2}$$

In [17], using previous knowlede in the context of QCD [18], it has been observed that $\gamma_S(\lambda)$ for large S is related to the anomalous dimension of cusped Maldacena-Wilson loops. The expectation value of such a Wilson loop diverges if parts of it are light-like, thus it has to be regulated by introducing IR and UV cutoffs L and ϵ

$$\langle \mathcal{W}[\mathcal{C}_{\text{cusp}}] \rangle \sim e^{-\Gamma_{\text{cusp}}(\lambda,\gamma) \ln \frac{L}{\epsilon}} \xrightarrow{\gamma \to \infty} e^{-f(\lambda)|\gamma| \ln \frac{L}{\epsilon}}, \tag{3.4.3}$$

where γ is a boost angle in Minkowski signature and $\Gamma_{\text{cusp}}(\gamma, \lambda)$ is the angle and coupling dependent cusp anomaly function. In the limit of large λ the function $f(\lambda)$ is obtained as the coefficient of the logarithmic divergence which in this context is also known as scaling function. It is related to the anomalous dimension of twist two operators via [17]

$$\gamma_S(\lambda) \simeq 2 f(\lambda) \ln S, \quad (S \to \infty). \tag{3.4.4}$$

The correspondence (3.3.2) now tells us that it is possible to access the scaling function also via path integral calculations from the string theory side

by considering fluctuations around a certain vacuum that acts as a minimal surface conformally bounded by a cusped contour $\mathcal{C}_{\text{cusp}}$. The remarks in [17, 19] suggest that the factor $|\gamma| \ln(L/\epsilon)$ in (3.4.3) corresponds to the regulated area of a cusped string worldsheet and is thus related to the world volume of the string $V_2 = \int \mathrm{d}\tau \mathrm{d}\sigma$, leading to

$$\langle \mathcal{W}[\mathcal{C}_{\text{cusp}}] \rangle = Z_{\text{string}}[\mathcal{C}_{\text{cusp}}] e^{-\frac{f(\lambda)}{2}\frac{V_2}{4}}. \tag{3.4.5}$$

Semiclassical quantisation around such vacua allowed to compute the scaling function up to two loops in sigma-model perturbation theory (see e.g. [15])

$$f(g) = 4g - \frac{3\ln 2}{\pi} - \frac{K}{4\pi^2 g} + \mathcal{O}(g^{-2}), \quad g \equiv \frac{\sqrt{\lambda}}{4\pi}, \tag{3.4.6}$$

where $K \approx 0.916$ is the CATALAN constant. As mentioned, the scaling function is also known relying on the assumption of the integrability of $\mathcal{N} \geq 4$ SYM (see e.g. [20]) where it can be derived from the BES^2 equation for any finite values of g. Our main aim is to reproduce the scaling function in numerical simulations for the string model with path integral defined by (a suitable version of) (3.3.3).

3.5 The Green-Schwarz superstring action in AdS light-cone gauge

As mentioned in the previous section we can address the scaling function by considering fluctuations around suitable vacua with worldsheets bounded by a cusp. Therefore we chose to follow the approach presented in [15]. We hereby start from a GREEN-SCHWARZ type superstring in AdS light-cone gauge with fixed κ-symmetry, that was proposed in [22, 23]. This action contains terms quadratic and quartic in fermions and has a classical solution X_{cl} forming a null-cusp on the AdS boundary. Now one can consider fluctuations around this classical solution and use (3.3.2) and (3.3.3) to match the vacuum expectation value of a WILSON loop around a null-cusp which is related to the scaling function via (3.4.3)

$$\langle \mathcal{W}_{\text{cusp}} \rangle = \int \mathcal{D}\delta X \, \mathcal{D}\delta \Psi \; e^{-S_{\text{cusp}}[X_{\text{cl}} + \delta X, \delta \Psi]} = e^{-\frac{f(\lambda)}{2}\frac{V_2}{4}}. \tag{3.5.1}$$

Hereby S_{cusp} refers to the action expanded around the null-cusp solution X_{cl} and $\Psi_{\text{cl}} = 0$, whereas Ψ is an abbreviated notation for the fermionic quantities and δX and $\delta \Psi$ are fluctuation fields. In the following we want to sketch shortly how to derive the action S_{cusp}. We will be using the $AdS_5 \times S^5$

[2] BES stands for Beisert-Eden-Staudacher equation, which is an integral equation derived via a BETHE Ansatz in quantum integrability [21].

metric in the POINCARÉ patch ($\mu = 0, \ldots, 3;\ M = 1, \ldots, 6$)

$$\mathrm{d}s^2 = z^{-2}\left(\mathrm{d}x^\mu \mathrm{d}x_\mu + \mathrm{d}z^M \mathrm{d}z^M\right) = z^{-2}\left(\mathrm{d}x^\mu \mathrm{d}x_\mu + \mathrm{d}z^2\right) + \mathrm{d}u^M \mathrm{d}u^M, \quad (3.5.2)$$

$$x^\mu x_\mu = x^+ x^- + x^* x, \quad x^\pm = x^3 \pm x^0, \quad x = x^1 + ix^2, \quad (3.5.3)$$

$$z^M = z u^M, \quad u^M u^M = 1, \quad z = \left(z^M z^M\right)^{\frac{1}{2}} \equiv e^\phi. \quad (3.5.4)$$

Here x^μ, z are the local coordinates in the POINCARÉ patch of AdS_5 (see Appendix B.2) and $u^M \in \mathbb{R}^6$ are EUCLIDEAN coordinates restricted to the S^5 sphere by (3.5.4). In this case AdS_5 and S^5 have the same constant curvature radius $R = 1$. Starting point is the action from [5], which is a covariant κ-symmetric superstring action for a Type IIB superstring on $AdS_5 \times S^5$ background. It is a 2d σ-model on the coset superspace $\frac{SU(2,2|4)}{SO(4,1)\times SO(5)}$. Fixing κ-symmetry $\Gamma^+ \vartheta^I = 0$ with $(I = 1, 2)$ on the two 10d MAJORANA-WEYL GS spinors ϑ^M and choosing the conformally analogue gauge on the 2d metric

$$\sqrt{-h} h^{\alpha\beta} = \mathrm{diag}(-z^2, z^{-2}) \quad (3.5.5)$$

is leading to the light-cone gauge with a simple solution for x^+

$$x^+ = p^+ \tau \quad (3.5.6)$$

which can be imposed as an additional constraint to fix the 2d diffeomorphism invariance. The resulting action on $AdS_5 \times S^5$ is

$$S = g \int \mathrm{d}\tau \int \mathrm{d}\sigma\, \mathcal{L}, \qquad g \equiv \frac{\sqrt{\lambda}}{4\pi}, \quad (3.5.7)$$

$$\begin{aligned}\mathcal{L} = {} & \dot{x}^* \dot{x} + \left(\dot{z}^M + i p^+ z^{-2} z^N \eta_i \left(\rho^{MN}\right)^i{}_j \eta^j\right)^2 + i p^+ \left(\theta^i \dot{\theta}_i + \eta^i \dot{\eta}_i + \theta_i \dot{\theta}^i + \eta_i \dot{\eta}^i\right) \\ & - (p^+)^2 z^{-2} \left(\eta^2\right)^2 - z^{-4}\left(x'^* x' + z'^M z'^M\right) \\ & - 2\Big[p^+ z^{-3} \eta^i \rho^M_{ij} z^M \left(\theta'^j - i z^{-1} \eta^j x'\right) + p^+ z^{-3} \eta_i \left(\rho^\dagger_M\right)^{ij} z^M \left(\theta'_j + i z^{-1} \eta_j x'^*\right)\Big],\end{aligned}$$

where we defined $\eta^2 \equiv \eta^i \eta_i$. The six 4×4 matrices ρ^M and their properties are stated in Appendix C. We also introduced the fields η_i, θ_i $(i = 1, \ldots, 4)$ which are complex GRASSMANN variables with $\eta^i \equiv (\eta_i)^\dagger, \theta^i \equiv (\theta_i)^\dagger$. They are the remnants of the original two 10d MAJORANA-WEYL GS spinors and transform in the fundamental representation of $SU(4)$. We will also refer to them as fermions due to their GRASSMANN-odd properties. The action is at most quartic in the fermions and the factors of p^+ can be absorbed by a rescaling of the selfsame and therefore we can set $p^+ = 1$. To get a real-valued BOLTZMANN factor e^{-S_E} in the path integral we perform a WICK rotation $\tau \to -i\tau$, $p^+ \to i p^+$ and after setting $p^+ = 1$ we obtain the

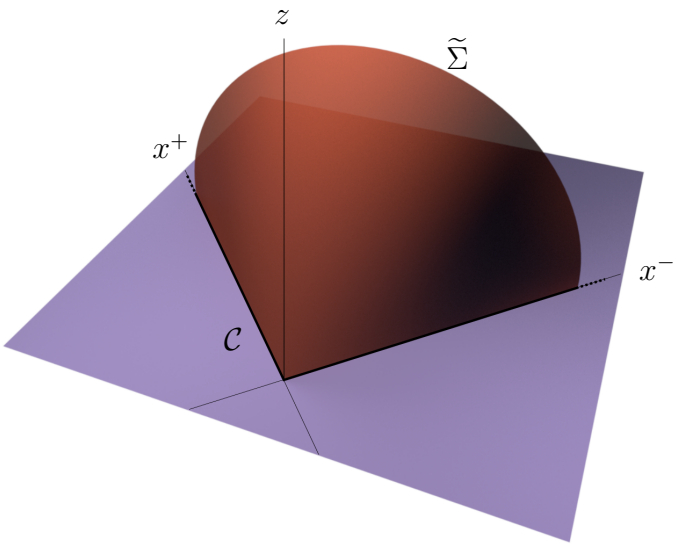

Figure 3.5.1 Visualisation of the string worldsheet in the AdS_3 subspace (which is orthogonal to the coordinates x, x^*). For $z \to 0$ the embedding of the string worldsheet $\widetilde{\Sigma}$ is bounded by a cusped contour $\mathcal{C}$ closed at infinity.

EUCLIDEAN action

$$S_{\mathrm{E}} = g \int \mathrm{d}\tau \int \mathrm{d}\sigma \, \mathcal{L}_{\mathrm{E}}, \tag{3.5.8}$$

$$\begin{aligned}\mathcal{L}_{\mathrm{E}} = {} & \dot{x}^* \dot{x} + \left(\dot{z}^M + i z^{-2} z^N \eta_i \left(\rho^{MN}\right)^i{}_j \eta^j\right)^2 + i\left(\theta^i \dot{\theta}_i + \eta^i \dot{\eta}_i + \theta_i \dot{\theta}^i + \eta_i \dot{\eta}^i\right) \\ & - z^{-2}\left(\eta^2\right)^2 + z^{-4}\left(x'^* x' + z'^M z'^M\right) \\ & + 2i\left[z^{-3}\eta^i \rho^M_{ij} z^M \left(\theta'^j - i z^{-1} \eta^j x'\right) + z^{-3}\eta_i \left(\rho^\dagger_M\right)^{ij} z^M \left(\theta'_j + i z^{-1} \eta_j x'^*\right)\right],\end{aligned}$$

As mentioned, this EUCLIDEAN superstring action has the simple classical solution of a null-cusp, given by

$$x^+ = \tau, \quad x^- = -\frac{1}{2\sigma}, \quad x^1 = x^2 = 0, \quad z = \sqrt{-2x^+x^-} = \sqrt{\frac{\tau}{\sigma}}, \tag{3.5.9}$$

$\tau, \sigma \in (0, \infty)$.

For $z \to 0$ we approach the AdS boundary and therefore the regime of $\mathcal{N} = 4$ SYM (see also Figure 3.5.1 for a visualization for the cusped contour).

The curve proceeding at the boundary can be parametrised by

$$\begin{aligned} \mathcal{C}_{\text{cusp}} \quad : \quad (-\infty,\infty) \quad &\longrightarrow \quad \mathbb{R}^{4,1} \\ s \quad &\longrightarrow \quad x^1 = x^2 = 0, \\ & \qquad x^+ = \begin{cases} -s & s<0, \\ 0 & \text{else}, \end{cases} \\ & \qquad x^- = \begin{cases} s & s>0, \\ 0 & \text{else}. \end{cases} \end{aligned} \tag{3.5.10}$$

To arrive at the form of (3.5.1) with a fluctuation action S_{cusp}, we need to expand S_{E} around the null-cusp background (3.5.9). We therefore choose the field fluctuations to be

$$x = \sqrt{\frac{\tau}{\sigma}}\tilde{x}, \quad z^M = \sqrt{\frac{\tau}{\sigma}}\tilde{z}^M, \quad \theta_i = \frac{1}{\sqrt{\sigma}}\tilde{\theta}_i, \quad \eta_i = \frac{1}{\sqrt{\sigma}}\tilde{\eta}_i. \tag{3.5.11}$$

With a transition to the new worldsheet coordinates $(\tau,\sigma) \to (t,s) = (\ln\tau, \ln\sigma)$ the fluctuation action has no direct t or s dependence

$$S_{\text{cusp}} = g\int \mathrm{d}t \int \mathrm{d}s\, \mathcal{L}_{\text{cusp}} \tag{3.5.12}$$

$$\begin{aligned} \mathcal{L}_{\text{cusp}} = {} & \left|\partial_t\tilde{x} + \tfrac{1}{2}\tilde{x}\right|^2 + \frac{1}{\tilde{z}^4}\left|\partial_s\tilde{x} - \tfrac{1}{2}\tilde{x}\right|^2 + \left(\partial_t\tilde{z}^M + \frac{1}{2}\tilde{z}^M + \frac{i}{\tilde{z}^2}\tilde{z}_N\tilde{\eta}_i\big(\rho^{MN}\big)^i{}_j\tilde{\eta}^j\right)^2 \\ & + \frac{1}{\tilde{z}^4}\left(\partial_s\tilde{z}^M - \tfrac{1}{2}\tilde{z}^M\right)^2 + i\left(\tilde{\theta}^i\partial_t\tilde{\theta}_i + \tilde{\eta}^i\partial_t\tilde{\eta}_i + \tilde{\theta}_i\partial_t\tilde{\theta}^i + \tilde{\eta}_i\partial_t\tilde{\eta}^i\right) - \frac{1}{\tilde{z}^2}\left(\tilde{\eta}^2\right)^2 \\ & + \frac{2i}{\tilde{z}^3}\tilde{z}^M\tilde{\eta}^i\left(\rho^M\right)_{ij}\left(\partial_s\tilde{\theta}^j - \frac{1}{2}\tilde{\theta}^j - \frac{i}{\tilde{z}}\tilde{\eta}^j\left(\partial_s\tilde{x} - \tfrac{1}{2}\tilde{x}\right)\right) \\ & + \frac{2i}{\tilde{z}^3}\tilde{z}^M\tilde{\eta}_i\left(\rho_M^\dagger\right)^{ij}\left(\partial_s\tilde{\theta}_j - \frac{1}{2}\tilde{\theta}_j + \frac{i}{\tilde{z}}\tilde{\eta}_j + \frac{i}{\tilde{z}}\tilde{\eta}^j\left(\partial_s\tilde{x} - \tfrac{1}{2}\tilde{x}\right)^*\right). \end{aligned}$$

In the following we will drop the tilde notation for convenience. We also want to remark that there has been no truncation applied and this is still the full fluctuation action and therefore perfectly valid for a further application on non-perturbative calculations. In a previous step we set the light-cone momentum $p^+ = 1$ for simplicity, but since p^+ actually is a dimensionfull quantity we will insert a mass scale parameter m that is also necessary for a later renormalization on the lattice and therefore change

$$\partial_t x + \frac{1}{2}x \to \partial_t x + \frac{m}{2}, \qquad \partial_t z^M + \frac{1}{2}z^M \to \partial_t z^M + \frac{m}{2}z^M \tag{3.5.13}$$

and in the same way also the terms with spacial derivatives.

3.6 Symmetries of the fluctuation action

In [23] it was presented, that the general κ-symmetry light-cone fixed action possesses several symmetries. Two fundamental ones, which are also inherited by the fluctuation action (3.5.12) in its gauge fixed status, are global symmetries.

- At first a $U(1) \sim SO(2)$ symmetry which rotates the x and x^* coordinate fields orthogonal to the other AdS_5 coordinates, which therefore does not affect the classical solution. In order for the action to be invariant, also the fermions need to be shifted with the following transformations and the infinitesimal parameter ϵ

$$\begin{aligned} \delta x &= e^{i\epsilon}\, x, & \delta\eta_i &= e^{i\frac{\epsilon}{2}}\, \eta_i, & \delta\theta_i &= e^{-i\frac{\epsilon}{2}}\, \theta_i, \\ \delta x^* &= e^{-i\epsilon}\, x^*, & \delta\eta^i &= e^{-i\frac{\epsilon}{2}}\, \eta^i, & \delta\theta^i &= e^{i\frac{\epsilon}{2}}\, \theta^i. \end{aligned} \tag{3.6.1}$$

- The other symmetry is an $SU(4) \sim SO(6)$, which concerns the z^M fields and is inherited after gauge fixing due to the S^5 structure. By introducing an infinitesimal $SU(4)$ rotation $\epsilon^i{}_j$ the global symmetry transformations are given by

$$\begin{gathered} \delta z^M = -\frac{1}{2}\epsilon^i{}_j (\rho^{MN})^j{}_i z^N \\ \delta\theta^i = \epsilon^i{}_j \theta^j, \quad \delta\theta_i = -\theta_j \epsilon^i{}_j, \quad \delta\eta^i = \epsilon^i{}_j \eta^i, \quad \delta\eta_i = -\eta_i \epsilon^i{}_j. \end{gathered} \tag{3.6.2}$$

  Hereby one can see that the z^M transform in the vector representation and the $\{\eta^i, \theta^i\}$ and $\{\eta_i, \theta_i\}$ in the fundamental and anti-fundamental representation of $SU(4)$, respectively.

3.7 Perturbative 1-loop free energy

Here we want to point out a quick check that fluctuations around the previously derived vacuum lead to the correct solution of (3.4.6). We therefore want to reproduce the constant $\frac{3\ln 2}{\pi}$ term in $f(g)$. We know from (3.4.5) that we can write

$$Z_{\text{string}} = e^{-\frac{1}{8}f(\lambda)V_2} \equiv e^{-\Gamma(\lambda)}, \quad V_2 = \int \mathrm{d}t \int \mathrm{d}s, \tag{3.7.1}$$

where we define

$$\Gamma = \Gamma^{(0)} + \Gamma^{(1)} + \Gamma^{(2)} + \cdots = \frac{1}{8} f(\lambda) V_2. \tag{3.7.2}$$

Thereby $\Gamma^{(0)} = S_{\text{E}}[X_{\text{cl}}, \Psi = 0]$ is the value of the classical action on the solution and $\Gamma^{(1)}, \Gamma^{(2)}, \ldots$ are quantum corrections. The scaling function can be expanded in the following way

$$f(g) = g\left[a_0 + \frac{a_1}{g} + \frac{a_2}{g^2} + \cdots\right]. \tag{3.7.3}$$

In [15] the 1-loop fluctuation coefficient a_1 has bee calculated via $\Gamma^{(1)} = -\ln Z^{(1)}$, where $Z^{(1)}$ is the exponential of the truncated fluctuation action that has only quadratic field contributions. The LAGRANGIAN can therefore be written as a matrix-vector product with fermionic and bosonic matrix

operators $\hat{D}_{\mathrm{F}}$ and $\hat{D}_{\mathrm{B}}$. The 1-loop approximation of the path integral can therefore be written as[3] (with $p^2 = (p_0)^2 + (p_1)^2$)

$$\begin{aligned}\Gamma^{(1)} &= \frac{1}{2}\ln\frac{\operatorname{Det}\hat{D}_{\mathrm{B}}}{\operatorname{Det}\hat{D}_{\mathrm{F}}} = \frac{V_2}{2}\int\frac{\mathrm{d}^2p}{(2\pi)^2}\ \ln\left[\frac{\det D_{\mathrm{B}}(p)}{\det D_{\mathrm{F}}(p)}\right] \\ &= \frac{V_2}{2}\int\frac{\mathrm{d}^2p}{(2\pi)^2}\ \ln\left[\frac{(p^2+m^2)\left(p^2+\frac{m^2}{2}\right)^2(p^2)^5}{\left(p^2+\frac{m^2}{4}\right)^8}\right] = -\frac{3\ln 2}{\pi}\frac{V_2}{8}m^2,\end{aligned} \tag{3.7.4}$$

leading to the correct 1-loop coefficient for $f(g)$ with $m = 1$.

[3]With $\operatorname{Det}\hat{O}$ we hereby mean the full infinite dimensional determinant in the sense of

$$\ln\operatorname{Det}\hat{O} = \operatorname{Tr}\ln\hat{O} = \int\mathrm{d}^d s\langle s|\operatorname{tr}\ln\hat{O}|s\rangle = \int\mathrm{d}^d s\ln[\det O(s)],$$

where tr and det refer to the regular trace and determinant if $\hat{O}$ is a matrix of operators and here $|s\rangle$ is an eigenbase of the operator $\hat{O}$.

4 Towards the lattice simulation

With the current status of the action (3.5.12) we could almost start to discretize the operators and fields, at least for the bosonic part this would not be a problem. For the fermions however this is not so straight forward. In order to include the fermionic contribution into the weight factor of the path integral like explained in section 2.3.3 one needs to integrate out the GRASSMANN variables to result into a PFAFFIAN or determinant of a fermionic operator. As presented in Appendix A.2 this is only possible if the fermions appearing are of quadratic order. But in the fluctuation action (3.5.12) also quartic contributions of fermions emerge, which have to be linearized first with help of a HUBBARD-STRATONOVICH transformation.[1]

4.1 Linearization of fermionic contributions

4.1.1 Naive approach and sign problem

The only quartic interactions are coming from the η fields and we can write this part of the action as

$$S_4^{\mathrm{F}}[\eta_i, \eta^i] = g \int \mathrm{d}t\mathrm{d}s \left[-\frac{1}{z^2} \left(\eta^2\right)^2 + \left(\frac{i}{z^2} z_N \eta_i \left(\rho^{MN}\right)^i{}_j \eta^j \right)^2 \right]. \tag{4.1.1}$$

In the path integral representation the EUCLIDEAN action contributes within an exponential $e^{-S_{\mathrm{E}}}$. By performing a naive HUBBARD-STATONOVICH transformation on this exponential we can reduce the four-fermion contributions to quadratic YUKAWA terms whereas we have to introduce 7 bosonic real auxiliary fields ϕ and ϕ^N

$$\begin{aligned} &\exp\left\{ -g \int \mathrm{d}t\mathrm{d}s \left[-\tfrac{1}{z^2} \left(\eta^2\right)^2 + \left(\tfrac{i}{z^2} z_N \eta_i \left(\rho^{MN}\right)^i{}_j \eta^j \right)^2 \right] \right\} \\ &\quad \sim \int \mathcal{D}\phi \mathcal{D}\phi^{\mathcal{M}} \exp\left\{ -g \int \mathrm{d}t\mathrm{d}s \left[\tfrac{1}{2}\phi^2 + \tfrac{\sqrt{2}}{z}\phi\eta^2 + \tfrac{1}{2}(\phi^M)^2 \right.\right. \\ &\qquad \left.\left. - i\tfrac{\sqrt{2}}{z^4}\phi_M \left(i\eta_i (\rho^{MN})^i{}_j \eta^j \right) z_N \right] \right\}. \end{aligned} \tag{4.1.2}$$

[1] See Appendix A.2 for details

Here we can notice that the second term appears to be complex, since the $SO(6)$ matrix in parenthesis is hermitian (with respect to the indices M, N)

$$\left(i\,\eta_i\big(\rho^{MN}\big)^i{}_j\eta^j\right)^\dagger = i\,\eta_j\big(\rho^{MN}\big)^j{}_i\eta^i, \tag{4.1.3}$$

where we have used (C.0.6). As discussed in section 2.3.4 this complex phase in the weight function is potentially leading to a non treatable sign problem. We therefore chose to make a field redefinition that circumvents the appearance of a complex phase during the HS transformation.

4.1.2 Alternative field redefinition

By using the identities for the $SO(6)$ matrices stated in Appendix C we can rewrite the second term in the Lagrangian of (4.1.1) as

$$\left(i\,\eta_i(\rho^{MN})^i{}_j n^N\eta^j\right)^2 = -3(\eta^2)^2 + 2\eta_i(\rho^N)^{ik}n_N\eta_k\eta^j(\rho^L)_{jl}n_L\eta^l, \tag{4.1.4}$$

where we defined $n^N = \frac{z^N}{z}$. This leads to the Lagrangian

$$\mathcal{L}_4 = \frac{1}{z^2}\left(-4\,(\eta^2)^2 + 2\left|\eta_i(\rho^N)^{ik}n_N\eta_k\right|^2\right). \tag{4.1.5}$$

In order to circumvent the sign problem the second term needs to be negative. To achieve this we define new fields[2]

$$\Sigma_i^j = \eta_i\eta^j \qquad \tilde{\Sigma}_j^i = (\rho^N)^{ik}n_N(\rho^L)_{jl}n_L\eta_k\eta^l. \tag{4.1.6}$$

with this new definitions it is simple to check that

$$\Sigma_i^j\Sigma_j^i = -(\eta^2)^2 \quad \tilde{\Sigma}_i^j\tilde{\Sigma}_j^i = -(\eta^2)^2 \quad \Sigma_j^i\tilde{\Sigma}_i^j = -\left|\eta_i(\rho^N)^{ik}n_N\eta_k\right|^2. \tag{4.1.7}$$

With this we then define

$$\Sigma_{\pm i}{}^j = \Sigma_i^j \pm \tilde{\Sigma}_i^j \tag{4.1.8}$$

and find

$$\Sigma_{\pm i}{}^j\Sigma_{\pm j}{}^i = -2(\eta^2)^2 \mp 2\left|\eta_i(\rho^N)^{ik}n_N\eta_k\right|^2. \tag{4.1.9}$$

We can thus substitute the new fields into the Lagrangian and obtain

$$\mathcal{L}_4 = \frac{1}{z^2}\left(-4\,(\eta^2)^2 \mp 2(\eta^2)^2 \mp \Sigma_{\pm i}{}^j\Sigma_{\pm j}{}^i\right), \tag{4.1.10}$$

where we only need to select the right sign in the field definition to overcome the sign problem, which is leading to

$$\mathcal{L}_4 = \frac{1}{z^2}\left(-6\,(\eta^2)^2 - \Sigma_{+i}{}^j\Sigma_{+j}{}^i\right). \tag{4.1.11}$$

[2]Where we actually set $\Sigma_i{}^j = \eta_i\eta^j$, then defined $\Sigma^i{}_j \equiv (\Sigma_i{}^j)^* = \Sigma_j{}^i$ to emphasize the notation Σ_i^j and equivalent for $\tilde{\Sigma}$.

If we then perform a HS transformation there will be no complex phase. The HS transformation yields

$$-\frac{6}{z^2}(\eta^2)^2 \to \frac{12}{z}\eta^2\phi + 6\phi^2, \tag{4.1.12}$$

where a single bosonic field was introduced like in the naive case. And further

$$-\frac{1}{z^2}\Sigma_+{}^i_j\Sigma_+{}^j_i \to \frac{2}{z}\Sigma_+{}^i_j\phi^j_i + \phi^i_j\phi^j_i \qquad \text{with} \qquad \left(\phi^i_j\right)^* = \phi^j_i\,. \tag{4.1.13}$$

Here the collection of fields ϕ^i_j can be thought of as a complex hermitian matrix with 16 real free parameters. We find it convenient to rescale the field $\phi \to \phi/\sqrt{6}$, to get rid of the pre factor of 6 in (4.1.12). After reinserting the old fields for Σ_+ we can conclude that

$$\mathcal{L}_4 \to \frac{12}{z}\eta^2\phi + \phi^2 + \frac{2}{z}\eta_j\phi^j_i\eta^i + \frac{2}{z}(\rho^N)^{ik}n_N\eta_k\phi^j_i(\rho^L)_{jl}n_L\eta^l + \phi^i_j\phi^j_i\,, \tag{4.1.14}$$

and we can write the full Lagrangian as

$$\begin{aligned}\mathcal{L}_{\text{cusp}} = &\left|\partial_t x + \frac{m}{2}x\right|^2 + \frac{1}{z^4}\left|\partial_s x - \frac{m}{2}x\right|^2 + \left(\partial_t z^M + \frac{m}{2}z^M\right)^2 \\ &+ \frac{1}{z^4}\left(\partial_s z^M - \frac{m}{2}z^M\right)^2 + \phi^2 + \operatorname{tr}\left(\tilde{\phi}\,\tilde{\phi}^\dagger\right) + \Psi^T\mathcal{O}_{\text{F}}\,\Psi\,.\end{aligned} \tag{4.1.15}$$

Hereby we defined the fermionic vector $\Psi \equiv (\theta^i, \theta_i, \eta^i, \eta_i)$ as well as the auxiliary matrix $\tilde{\phi} = (\tilde{\phi}_{ij}) \equiv \phi^i_j$. We used partial integration and the properties of the Grassmann numbers and $SO(6)$ matrices to write the fermionic contribution in a matrix-vector notation. The 16×16 fermionic operator is hereby represented as 4×4 block matrix

$$\mathcal{O}_{\text{F}} = \begin{pmatrix} 0 & i\mathbb{1}_4\partial_t & -i\rho^M\left(\partial_s + \frac{m}{2}\right)\frac{z^M}{z^3} & 0 \\ i\mathbb{1}_4\partial_t & 0 & 0 & -i\rho^\dagger_M\left(\partial_s + \frac{m}{2}\right)\frac{z^M}{z^3} \\ i\frac{z^M}{z^3}\rho^M\left(\partial_s - \frac{m}{2}\right) & 0 & 2\frac{z^M}{z^4}\rho^M\left(\partial_s x - m\frac{x}{2}\right) & i\mathbb{1}_4\partial_t - A^T \\ 0 & i\frac{z^M}{z^3}\rho^\dagger_M\left(\partial_s - \frac{m}{2}\right) & i\mathbb{1}_4\partial_t + A & -2\frac{z^M}{z^4}\rho^\dagger_M\left(\partial_s x^* - m\frac{x}{2}^*\right) \end{pmatrix}, \tag{4.1.16}$$

where

$$A = -\frac{\sqrt{6}}{z}\phi\mathbb{1}_4 + \frac{1}{z}\tilde{\phi} + \frac{1}{z^3}\rho^*_N\tilde{\phi}^T\rho^L z^N z^L + \mathrm{i}\frac{z^N}{z^2}\rho^{MN}\partial_t z^M. \tag{4.1.17}$$

The auxiliary matrix $\tilde{\phi}$ is constructed from 16 real auxiliary fields ϕ_I ($I = 1,\ldots,16$) in the following way

$$\tilde{\phi} = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{2}\phi_{13} & \phi_1 + i\phi_2 & \phi_3 + i\phi_4 & \phi_5 + i\phi_6 \\ \phi_1 - i\phi_2 & \sqrt{2}\phi_{14} & \phi_7 + i\phi_8 & \phi_9 + i\phi_{10} \\ \phi_3 - i\phi_4 & \phi_7 - i\phi_8 & \sqrt{2}\phi_{15} & \phi_{11} + i\phi_{12} \\ \phi_5 - i\phi_6 & \phi_9 - i\phi_{10} & \phi_{11} - i\phi_{12} & \sqrt{2}\phi_{16} \end{pmatrix}, \tag{4.1.18}$$

so that we have the simple expression

$$\operatorname{tr}\left(\tilde{\phi}\,\tilde{\phi}^\dagger\right) = \sum_{I=1}^{16}(\phi_I)^2 \equiv (\phi_I)^2\,. \tag{4.1.19}$$

4.1.3 Matrix properties

The fermion matrix obeys some fundamental symmetries that shall be summarized in this section. Since $\mathcal{O}_\mathrm{F}$ is acting as a bilinear together with the anticommuting Grassmann fields, it is clear that the matrix representation of $\mathcal{O}_\mathrm{F}$ needs to be skew-symmetric

$$\mathcal{O}_\mathrm{F}^\mathrm{T} = -\mathcal{O}_\mathrm{F}. \tag{4.1.20}$$

It further possesses a global $U(1)$ and $SO(6)$ symmetry. The $U(1)$ symmetry manifests itself through the fact that certain blocks of $\mathcal{O}_\mathrm{F}$ are zero. As we saw from (3.6.1) fermions transform under $U(1)$ according to a certain charge q

$$\psi \to e^{iq\alpha}\psi. \tag{4.1.21}$$

Therefore only fermions with complementary charges are allowed to couple in order to respect the $U(1)$ symmetry, and the blocks that lead to other couplings need to be zero. The $SO(6)$ symmetry requires the 4×4 block structure and that each block is built from the $SO(6)$ invariant structures: $\mathbb{1}_4$, $\rho^M u^M$, $\rho_M^\dagger u^M$. The fermion matrix obeys also another constraint which is reminiscent of the γ_5-hermiticity in lattice QCD [7]

$$\mathcal{O}_\mathrm{F}^\dagger = \Gamma_5 \mathcal{O}_\mathrm{F} \Gamma_5, \tag{4.1.22}$$

where Γ_5 is the following unitary, antihermitian matrix

$$\Gamma_5 = \begin{pmatrix} 0 & \mathbb{1}_4 & 0 & 0 \\ -\mathbb{1}_4 & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{1}_4 \\ 0 & 0 & -\mathbb{1}_4 & 0 \end{pmatrix}, \qquad \Gamma_5^\dagger \Gamma_5 = \mathbb{1}_{16}, \quad \Gamma_5^\dagger = -\Gamma_5. \tag{4.1.23}$$

A general skew-symmetric block matrix M that is Γ_5-hermitian needs to have the structure

$$M = \begin{pmatrix} d_1 & a & b & c \\ -a^\mathrm{T} & -d_1^\dagger & -c^* & b^* \\ -b^\mathrm{T} & c^\dagger & d_2 & f \\ -c^\mathrm{T} & -b^\dagger & -f^\mathrm{T} & -d_2^\dagger \end{pmatrix}, \qquad d_i = -d_i^\mathrm{T}, \quad a = a^\dagger, \quad f = f^\dagger. \tag{4.1.24}$$

We can use the two properties (4.1.20) and (4.1.22) to ensure the absence of a complex phase in the determinant

$$\begin{aligned} \det\left(\mathcal{O}_\mathrm{F}\right)^* &= \det\left(\mathcal{O}_\mathrm{F}^\dagger\right) = \det\left(\Gamma_5 \mathcal{O}_\mathrm{F} \Gamma_5\right) \\ &= \det\left(\Gamma_5\right)^2 \det\left(\mathcal{O}_\mathrm{F}\right) \\ &= \det\left(\mathcal{O}_\mathrm{F}\right) \end{aligned} \tag{4.1.25}$$

and thereby follows that $\det \mathcal{O}_\mathrm{F} \in \mathbb{R}$. For the Pfaffian of $\mathcal{O}_\mathrm{F}$ to be nonnegative we require that $\det \mathcal{O}_\mathrm{F}$ is positive and factorizable into two equivalent terms, so that

$$\det \mathcal{O}_\mathrm{F} = \mathrm{Pf}\left(\mathcal{O}_\mathrm{F}\right)^2. \tag{4.1.26}$$

Therefore we want to examine the spectrum of $\mathcal{O}_\mathrm{F}$. Assuming that λ is an eigenvalue of $\mathcal{O}_\mathrm{F}$ and $P(\lambda)$ is the characteristic polynomial we can prove

$$\begin{aligned} P(\lambda) &= \det(\mathcal{O}_\mathrm{F} - \lambda\mathbb{1}) = \det(\Gamma_5(\mathcal{O}_\mathrm{F} - \lambda\mathbb{1})\Gamma_5) \\ &= \det(\mathcal{O}_\mathrm{F}^\dagger + \lambda\mathbb{1}) = \det(\mathcal{O}_\mathrm{F} + \lambda^*\mathbb{1})^* \\ &= P(-\lambda^*)^*, \end{aligned} \tag{4.1.27}$$

and thereby see that if λ is an eigenvalue, then also $-\lambda^*$ is an eigenvalue. Since $\mathcal{O}_\mathrm{F}$ is skew-symmetric also $-\lambda$ and λ^* must be eigenvalues. So if for a discretized version $\hat{\mathcal{O}}_\mathrm{F}$ all these eigenvalues would be complex with non-vanishing real and imaginary part we could write the determinant as

$$\det \hat{\mathcal{O}}_\mathrm{F} = \prod_{i=1}^{N} |\lambda_i|^2 |\lambda_i|^2 \tag{4.1.28}$$

and therefore

$$\mathrm{Pf}\, \hat{\mathcal{O}}_\mathrm{F} = \pm \prod_{i=1}^{N} |\lambda_i|^2, \tag{4.1.29}$$

where $N = |\Lambda|/4$. Since the eigenvalues should behave like continuous functions along a HMC trajectory it should not be possible for the Pfaffian to change its sign throughout a trajectory. So if one chooses a starting configuration with positive Pfaffian it should remain nonnegative during the whole simulation and the Pfaffian should be a valid probability distribution. Yet it is not quite clear what happens if there are also purely real or imaginary eigenvalues appearing. If they come in the same kind of quartets then there should not be a problem, otherwise the behaviour is not fully understood yet. We therefore need to keep track of of the Pfaffian during simulation to legitimate its status as valid probability density.

4.1.4 Pseudofermionic weight function

Now since we have linearised fermionic contributions to quadratic order, we are able to integrate over the Grassmann fields in the partition function

$$Z = \int \mathcal{D}x\, \mathcal{D}x^*\, \mathcal{D}z^N\, \mathcal{D}\phi\, \mathcal{D}\phi_I\, \mathcal{D}\Psi\; e^{-S}\,, \tag{4.1.30}$$

where we will split $S = S_\mathrm{B} + S_\mathrm{F}$ into its bosonic (S_B) and fermionic (S_F) contributions with

$$\begin{aligned} S_\mathrm{B} = g \int \mathrm{d}t\mathrm{d}s\, &\left|\partial_t x + \frac{m}{2}x\right|^2 + \frac{1}{z^4}\left|\partial_s x - \frac{m}{2}x\right|^2 + \left(\partial_t z^M + \frac{m}{2}z^M\right)^2 \\ &+ \frac{1}{z^4}\left(\partial_s z^M - \frac{m}{2}z^M\right)^2 + \phi^2 + (\phi_I)^2\,, \end{aligned} \tag{4.1.31}$$

$$S_\mathrm{F} = g \int \mathrm{d}t\mathrm{d}s\; \Psi^T \mathcal{O}_\mathrm{F}\, \Psi\,.$$

As motivated in section A.2 the GRASSMANN integral over Ψ will result in a PFAFFIAN $\operatorname{Pf}\mathcal{O}_{\mathrm{F}}$. To include the PFAFFIAN into the weight function we have to rewrite it in terms of pseudofermions ξ as emphasized in section 2.3.3. To legitimately apply this procedure we need the PFAFFIAN to be real and non-negative. By our alternative approach to linearization we made sure to exclude any potential phase ambiguities. As we could see from the previous section we are convinced that the PFAFFIAN can be treated as a positive real quantity which we will assume to be true in the following. For this reason, we proceed as in [24] and introduce pseudofermions ξ via

$$\int \mathcal{D}\Psi\; e^{-S_{\mathrm{F}}} = \operatorname{Pf}\mathcal{O}_{\mathrm{F}} = \left(\det \mathcal{O}_{\mathrm{F}}\, \mathcal{O}_{\mathrm{F}}^{\dagger}\right)^{\frac{1}{4}} = \int \mathcal{D}\xi\, \mathcal{D}\xi^{\dagger}\; e^{-S_{\xi}}\,, \tag{4.1.32}$$

where

$$S_{\xi} = g \int \mathrm{d}t\mathrm{d}s\; \xi^{\dagger} \left(\mathcal{O}_{\mathrm{F}}\, \mathcal{O}_{\mathrm{F}}^{\dagger}\right)^{-\frac{1}{4}} \xi\,, \tag{4.1.33}$$

and ξ is a collection of 16 complex bosonic scalar fields. But before we can go any further we need to discretize the action with help of the methods introduced in section 2.1.

4.2 Discretizing the action

In the previous steps we have constructed a LAGRANGIAN fitting to our problem and modified terms to be able to apply a RHMC algorithm. To proceed with this task we need a discretized version of the bosonic action and the fermionic operator $\mathcal{O}_{\mathrm{F}}$.

4.2.1 Bosonic action

For the bosonic term this is quite easy. First we need to do a dimensional analysis of the fields in the action. In the simulation we can only deal with dimensionless fields. Since the action also needs to be dimensionless we can see that the fields x, x^* and z^M are dimensionless as preferred but the auxiliary fields are of dimension $[\phi] = 1/[a]$. We therefore do a redefinition of the discretized fields

$$a\phi(n) \to \phi(n), \qquad a\phi_I(n) \to \phi_I(n) \tag{4.2.1}$$

in order to have dimensionless quantities as well. We can now write the discretized version of the bosonic action in (4.1.31) as

$$\begin{aligned}\hat{S}_{\mathrm{B}} = g \sum_{n\in\Lambda} \Bigg[& \left| x(n+\hat{0}) + \left(\tfrac{M}{2}-1\right) x(n) \right|^2 + \frac{1}{[z(n)]^4} \left| x(n+\hat{1}) - \left(\tfrac{M}{2}+1\right) x(n) \right|^2 \\ & + \sum_{M=1}^{6} \Bigg\{ \left(z^M(n+\hat{0}) + \left(\tfrac{M}{2}-1\right) z^M(n) \right)^2 \\ & \qquad + \frac{1}{[z(n)]^4} \left(z^M(n+\hat{1}) - \left(\tfrac{M}{2}+1\right) z^M(n) \right)^2 \Bigg\} \\ & + \phi^2(n) + \sum_{I=1}^{16} [\phi_I(n)]^2 \Bigg],\end{aligned} \tag{4.2.2}$$

where we applied a simple forward derivative to the x, x^* and z^M fields and introduced the dimensionless lattice mass parameter $M = ma$.

4.2.2 Wilson term

Before discretizing the fermionic operator we have to think about the doubling problem arising through naively discretized first derivatives, discussed in subsection 2.2.2. The free fermionic operator (evaluated in the bosonic vacuum) represented in a momentum basis reads

$$K_{\mathrm{F}} = \begin{pmatrix} 0 & -p_0 \mathbb{1}_4 & \left(p_1 - i\frac{m}{2}\right) \rho^M u^M & 0 \\ -p_0 \mathbb{1}_4 & 0 & 0 & \left(p_1 - i\frac{m}{2}\right) \rho_M^\dagger u^M \\ -\left(p_1 + i\frac{m}{2}\right) \rho^M u^M & 0 & 0 & -p_0 \mathbb{1}_4 \\ 0 & -\left(p_1 + i\frac{m}{2}\right) \rho_M^\dagger u^M & -p_0 \mathbb{1}_4 & 0 \end{pmatrix}, \tag{4.2.3}$$

and has determinant

$$\det K_{\mathrm{F}} = \left(p_0^2 + p_1^2 + \frac{m^2}{4} \right)^8. \tag{4.2.4}$$

The fermionic propagators are proportional to the inverse of dynamic operators. It is therefore reasonable that the naive discretization (like in (2.2.12))

$$p_i \to \mathring{p}_i \equiv \frac{1}{a} \sin(p_i a) \tag{4.2.5}$$

will give rise to doublers. For this reason we would like to introduce a Wilson-like term that cancels the additional poles in the fermionic propagator. It should obey the following conditions:

- preserve the maximal amount of symmetries and relevant matrix properties,
- give the correct continuum limit for $a \to 0$,

- should not give rise to a complex phase.

Due to the properties of $\mathcal{O}_\mathrm{F}$ presented in subsection 4.1.3 we can see that there is only a small margin of variations that we can apply to the fermion matrix as a WILSON term and that respects the $U(1)$ and $SO(6)$ symmetries. In fact it was not possible to construct such an operator that also preserves relevant matrix properties like skew- and Γ_5-symmetry and also leads to the correct perturbative 1-loop coefficient in (3.4.6).
We therefore chose to explicitly break the $U(1)$ symmetry and introduce a WILSON-like operator on the diagonal blocks of $\mathcal{O}_\mathrm{F}$. In terms of the free fermion operator in momentum space this takes the form

$$\hat{K}_\mathrm{F} = \begin{pmatrix} W_+ & -\mathring{p}_0 \mathbb{1}_4 & \left(\mathring{p}_1 - i\frac{m}{2}\right) \rho^M u^M & 0 \\ -\mathring{p}_0 \mathbb{1}_4 & -W_+^\dagger & 0 & \left(\mathring{p}_1 - i\frac{m}{2}\right) \rho_M^\dagger u^M \\ -\left(\mathring{p}_1 + i\frac{m}{2}\right) \rho^M u^M & 0 & W_- & -\mathring{p}_0 \mathbb{1}_4 \\ 0 & -\left(\mathring{p}_1 + i\frac{m}{2}\right) \rho_M^\dagger u^M & -\mathring{p}_0 \mathbb{1}_4 & -W_-^\dagger \end{pmatrix}, \tag{4.2.6}$$

where

$$W_\pm = \frac{ra}{2} \left(\hat{p}_0^2 \pm i\hat{p}_1^2\right) \rho^M u^M, \qquad |r| = 1, \tag{4.2.7}$$

and similar to (2.2.16)

$$\hat{p}_i \equiv \frac{2}{a} \sin \frac{p_i a}{2}\,. \tag{4.2.8}$$

This leads to the analogue expression of (4.2.4)

$$\det \hat{K}_\mathrm{F} = \left(\mathring{p}_0^2 + \mathring{p}_1^2 + \frac{r^2 a^2}{4} \left(\hat{p}_0^4 + \hat{p}_1^4\right) + \frac{m^2}{4} \right)^8 . \tag{4.2.9}$$

If we substitute this into the denominator of (3.7.4) and apply the replacement $p_i^2 \to \hat{p}_i^2$ in the numerator, the discretized equivalent of the 1-loop free energy can be defined by

$$\Gamma^{(1)}_\mathrm{LAT} = -\ln Z^{(1)}_\mathrm{LAT} = \mathcal{I}(a). \tag{4.2.10}$$

With $r = 1$ and rescaled momentum integration over the first BRILLOUINE zone this results in

$$\begin{aligned} \mathcal{I}(a) = \frac{V_2}{2a^2} \int_{-\pi}^{\pi} \frac{\mathrm{d}^2 p}{(2\pi)^2} \Bigg\{ & 5 \ln \left[4 \Big(\sin^2 \frac{p_0}{2} + \sin^2 \frac{p_1}{2} \Big) \right] \\ & + 2 \ln \left[4 \Big(\sin^2 \frac{p_0}{2} + \sin^2 \frac{p_1}{2} + \frac{M^2}{8} \Big) \right] \\ & + \ln \left[4 \Big(\sin^2 \frac{p_0}{2} + \sin^2 \frac{p_1}{2} + \frac{M^2}{4} \Big) \right] \\ & - 8 \ln \left[4 \sin^4 \frac{p_0}{2} + \sin^2 p_0 + 4 \sin^4 \frac{p_1}{2} + \sin^2 p_1 + \frac{M^2}{4} \right] \Bigg\}. \end{aligned} \tag{4.2.11}$$

For a consistent discretization this should lead to the same result as (3.7.4) in the $a \to 0$ limit. And indeed a numerical integration of (4.2.11) yields

$$\Gamma^{(1)} = -\ln Z^{(1)} = \lim_{a\to 0} \mathcal{I}(a) = -\frac{3\ln 2}{8\pi}|\Lambda|M^2, \tag{4.2.12}$$

where we used that $V_2 = a^2|\Lambda| = a^2 LT$ and we are left with the expected result. Given the structure of the WILSON term in the vacuum it is quite natural to generalize it to the interacting case. The discretized momentum space operator therefore reads

$$\widetilde{\mathcal{O}}_{\mathrm{F}} = \begin{pmatrix} W_+ & -\mathring{p}_0 \mathbb{1}_4 & \left(\mathring{p}_1 - i\frac{m}{2}\right)\rho^M u^M & 0 \\ -\mathring{p}_0 \mathbb{1}_4 & -W_+^\dagger & 0 & \left(\mathring{p}_1 - i\frac{m}{2}\right)\rho_M^\dagger u^M \\ -\left(\mathring{p}_1 + i\frac{m}{2}\right)\rho^M u^M & 0 & 2\frac{z^M}{z^4}\rho^M(\partial_s x - \frac{m}{2}x) + W_- & -\mathring{p}_0 \mathbb{1}_4 \\ 0 & -\left(\mathring{p}_1 + i\frac{m}{2}\right)\rho_M^\dagger u^M & -\mathring{p}_0 \mathbb{1}_4 & -2\frac{z^M}{z^4}\rho_M^\dagger(\partial_s x^* - \frac{m}{2}x^*) - W_-^\dagger \end{pmatrix}, \tag{4.2.13}$$

with

$$W_\pm = \frac{ra}{2z^2}\left(\hat{p}_0^2 \pm i\hat{p}_1^2\right)\rho^M z^M, \tag{4.2.14}$$

where an additional $1/z$ factor is present for the purpose of improved stability during simulations. From (4.1.24) one can see that the added WILSON term respects the Γ_5-hermiticity and skew-symmetry which ensures the determinant to be real and positive.

4.2.3 Fermionic operator

By knowing the structure of the WILSON term we can finally discretize the fermionic operator and write it in terms of a single matrix by using the lexicographic index notation introduced in section 2.1. The discretized fermion matrix $\hat{\mathcal{O}}_{\mathrm{F}}$ is of size $16V \times 16V$ and we are going to subdivide it into 4 by 4 blocks of size $4V \times 4V$ as

$$\left(\hat{\mathcal{O}}_{\mathrm{F}}\right)_{16V\times 16V} = \left(\begin{array}{c|c|c|c} O_{4V\times 4V} & \cdots & \cdots & \cdots \\ \hline \vdots & \ddots & & \\ \hline \vdots & & \ddots & \\ \hline \vdots & & & \ddots \end{array}\right). \tag{4.2.15}$$

To build the block matrices we assume that for every lattice index $l, p = 0, \ldots, (V-1)$ we have a 4×4 matrix with indices $i, j = 1, \ldots, 4$ and emphasize the structure

$$O_{4\times 4}(V \times V) \longleftrightarrow O_{ij}(l, p). \tag{4.2.16}$$

One can map this to a $4V \times 4V$ matrix with global indices like

$$O_{4V\times 4V} \longleftrightarrow O_{AB}, \qquad A = 4l + i, \quad B = 4p + j. \tag{4.2.17}$$

The discretized fermion matrix is now given by

$$\hat{\mathcal{O}}_{\mathrm{F}} = \begin{pmatrix} \hat{W}_+ & i\bar{\Delta}_0^{\mathrm{A}} & -i\left(\vec{\Delta}_1^{Z} + \frac{M}{2}\bar{Z}\right) & 0 \\ i\bar{\Delta}_0^{\mathrm{A}} & -\hat{W}_+^{\dagger} & 0 & -i\left(\vec{\Delta}_1^{Z^\dagger} + \frac{M}{2}\bar{Z}^\dagger\right) \\ i\left(\bar{\Delta}_1^{Z} - \frac{M}{2}\bar{Z}\right) & 0 & 2\left(\bar{\Delta}_1^{x} - \frac{M}{2}\bar{Z}^{x}\right) + \hat{W}_- & i\bar{\Delta}_0^{\mathrm{A}} - \hat{A}^{\mathrm{T}} \\ 0 & i\left(\bar{\Delta}_1^{Z^\dagger} - \frac{M}{2}\bar{Z}^\dagger\right) & i\bar{\Delta}_0^{\mathrm{A}} + \hat{A} & 2\left(\bar{\Delta}_1^{x^*} - \frac{M}{2}\bar{Z}^{x^*}\right) - \hat{W}_-^{\dagger} \end{pmatrix}, \tag{4.2.18}$$

where we refer the reader to Appendix E for a detailed derivation of the single terms.

4.3 Applying the RHMC algorithm

Since the current status is a realization of discretized operators and fields that are also dimensionless, we can return to a discretized version of the equations (4.1.30-4.1.33) and implement a RHMC algorithm based on HMC algorithm introduced in section 2.3.3. There we described the algorithm by means of an inversed hermitian operator in the pseudofermionic action

$$\hat{S}_\xi = g\xi^\dagger \left(\hat{M}^\dagger \hat{M}\right)^{-1} \xi, \tag{4.3.1}$$

where we applied a matrix-vector notation in the sense of (2.1.10). In our present case we are instead faced with

$$\hat{S}_\xi = g\xi^\dagger \left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger \hat{\mathcal{O}}_{\mathrm{F}}\right)^{-\frac{1}{4}} \xi. \tag{4.3.2}$$

To treat this kind of matrix valued function one uses a rational approximation

$$\left(\hat{M}^\dagger \hat{M}\right)^{\rho} = \alpha_0 + \sum_{i=1}^{P} \frac{\alpha_i}{\hat{M}^\dagger \hat{M} + \beta_i \mathbb{1}}, \tag{4.3.3}$$

where α_i and β_i are constant coefficients. For predicted limits of the eigenvalues $\lambda_{\min}$ and $\lambda_{\max}$ of a matrix and of cause a given exponent ρ one can use a Remez algorithm to obtain the coefficients α_i and β_i up to some order P of accuracy of the approximation, valid for any matrix satisfying the spectral bounds.
For the implementation of the RHMC we need two sets of coefficients for two different approximations with $\rho = 1/8$ and $\rho = -1/4$, respectively. The requirement of $\rho = -1/4$ should be clear, but we also need an approximation with $\rho = 1/8$ to generate pseudofermionic fields[3]

$$\xi = \left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger \hat{\mathcal{O}}_{\mathrm{F}}\right)^{\frac{1}{8}} \vartheta \tag{4.3.4}$$

[3]Compare to the list of items in section 2.3.3.

distributed according to

$$\exp\left(-\vartheta^\dagger\vartheta\right) = \exp\left(-\xi^\dagger\left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}}\right)^{-\frac{1}{4}}\xi\right). \tag{4.3.5}$$

We use an order $P = 15$ approximation and the utilized values α_i and β_i can be found in Table 5.2.1. In order to state the full RHMC procedure we want to take a closer look at the pseudofermionic contribution to the bosonic force

$$F_m^\xi[\Phi] = \frac{\partial}{\partial\Phi_m}\left[\xi^\dagger\left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}}\right)^{-\frac{1}{4}}\xi\right], \quad \Phi_m = \left(x, x^*, z^N, \phi, \phi^I\right), \tag{4.3.6}$$

with $m = 1, \ldots, 25$. Inserting the rational approximation yields[4]

$$\begin{aligned} F_m^\xi[\Phi] &= -\sum_{i=1}^{P}\alpha_i\left(\frac{1}{\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}} + \beta_i\mathbb{1}}\xi\right)^\dagger\frac{\partial}{\partial\Phi_m}\left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}}\right)\left(\frac{1}{\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}} + \beta_i\mathbb{1}}\xi\right) \\ &= -\sum_{i=1}^{P}\alpha_i\left[\left(\hat{\mathcal{O}}_{\mathrm{F}}s_i\right)^\dagger\frac{\partial\hat{\mathcal{O}}_{\mathrm{F}}}{\partial\Phi_m}s_i + s_i^\dagger\frac{\partial\hat{\mathcal{O}}_{\mathrm{F}}^\dagger}{\partial\Phi_m}\hat{\mathcal{O}}_{\mathrm{F}}s_i\right], \end{aligned} \tag{4.3.7}$$

where $s_i = \left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}} + \beta_i\mathbb{1}\right)^{-1}\xi$ are interpreted as the solutions to the matrix equation

$$\left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}} + \beta_i\mathbb{1}\right)s^i = \xi, \qquad i = 1, \ldots, P\,. \tag{4.3.8}$$

To obtain all P solutions at once, we employ a *multi-shift conjugate gradient solver* adapted from the `openQCD` package[5] by Martin Lüscher. For the single terms of the matrix derivative $\partial\hat{\mathcal{O}}_{\mathrm{F}}/\partial\Phi_m$ we refer the reader to the Appendix **INSERT APP REF**. The single steps for the RHMC are therefore:

- **Pseudofermions**
  Generate the $16V$-dimensional pseudofermionic field $\xi = \left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger\hat{\mathcal{O}}_{\mathrm{F}}\right)^{\frac{1}{8}}\vartheta$, where ϑ is distributed according $\exp\left(-\vartheta^\dagger\vartheta\right)$.
- **Conjugate fields**
  For an initial boson configuration $\Phi^{(0)}$ generate $\Pi^{(0)}$ according to the GAUSSIAN distribution $\exp\left(-\frac{1}{2}\Pi^2\right)$.
- **Initial step**
  $\Pi_m^{(\frac{1}{2})} = \Pi_m^{(0)} - \frac{\epsilon}{2}F_m[\Phi]\Big|_{\Phi^{(0)}}$.
- **Intermediate step**
  Full steps for $j = 1, \ldots, n-1$
  $\Phi_m^{(j)} = \Phi_m^{(j-1)} + \Pi_m^{(j-\frac{1}{2})}, \quad \Pi_m^{(j+\frac{1}{2})} = \Pi_m^{(j-\frac{1}{2})} - \epsilon F_m[\Phi]\Big|_{\Phi^{(j)}}$.

[4] With help of the matrix-scalar derivative $\dfrac{\partial U^{-1}(x)}{\partial x} = -U^{-1}\dfrac{\partial U}{\partial x}U^{-1}$.

[5] `http://luscher.web.cern.ch/luscher/openQCD/`

- **Final step**
  $\Phi'_m = \Phi_m^{(n)} = \Phi_m^{(n-1)} + \Pi_m^{(n-\frac{1}{2})}, \quad \Pi'_m = \Pi_m^{(n)} = \Pi_m^{(n-\frac{1}{2})} - \frac{\epsilon}{2} F_m[\Phi]\Big|_{\Phi^{(n)}}$.

- **Monte Carlo step**
  Accept new configuration Φ' if a random number $r \in [0, 1)$ is smaller than

$$\exp\left(\frac{1}{2}\left(\Pi^2 - \Pi'^2\right) + S_{\mathrm{B}}[\Phi] - S_{\mathrm{B}}[\Phi'] + \vartheta^\dagger \vartheta - \xi^\dagger \left(\hat{\mathcal{O}}_{\mathrm{F}}^\dagger \hat{\mathcal{O}}_{\mathrm{F}}\right)^{-\frac{1}{4}} \xi\right) .$$

Hereby we have used

$$F_m[\Phi] = \frac{\partial S_{\mathrm{B}}[\Phi]}{\partial \Phi_m} + F_m^\xi[\Phi]. \tag{4.3.9}$$

5 Simulations and observables

In this chapter we will present some basic information on the implementation of the previously discussed algorithm and state the utilized parameters of the conducted simulations. Furthermore we need to discuss how to take the continuum limit of the observables of interest.

5.1 Implementation and the continuum limit

The executables for the Monte Carlo simulation are built from an implementation in the FORTRAN 95 standard and compiled with an Intel® `ifort` compiler[1]. For the lattice we deploy several sizes for the spatial extent $L = 8, 10, 12, 16, 24, 32$, whereas the temporal extent is always twice of the spatial one $T = 2L$ for an improved accuracy of the bosonic correlators. Thus we have a world volume of $V_2 = 2a^2L^2$. In the continuum model there are two "bare" parameters that determine its behaviour, the dimensionless coupling $g = \sqrt{\lambda}/4\pi$ and the mass scale m. To take the continuum limit it is necessary to set a line of constant physics when $a \to 0$ which is said to be the squared physical mass of the field excitations rescaled with the world volume

$$V_2 m_x^2 = \text{const.} \tag{5.1.1}$$

From a dimensional regularization scheme it is possible to find the corrections to the masses of the bosonic fields x, x^* which read [25]

$$m_x^2(g) = \frac{m^2}{2}\left(1 - \frac{1}{8g} + \mathcal{O}(g^{-2})\right). \tag{5.1.2}$$

Together with (5.1.1) this leads to

$$\frac{V_2 m^2}{2} = (LM)^2 = \text{const}, \tag{5.1.3}$$

where $M = ma$ is the dimensionless lattice mass scale. The equality (5.1.3) relies on the hypothesis that g is not (infinitely) renormalized. Further the validity of (5.1.2) in the discretized model needs to be verified in order the physical masses undergo only a finite renormalization. This claim is supported by studying x, x^* correlators where indeed no presence $(1/a)$

[1] From the Intel® Parallel Studio XE 2015.

divergences in the m_x^2/m^2 ratios can be found. Also for the large g region they reach their expected continuum value of $1/2$. Having this in mind and also the result of the perturbative 1-loop free energy (3.7.4), we assume no further presence of a scale in the discretized model other than the lattice spacing a. Therefore any expectation value of an observable $\langle F_{\mathrm{LAT}} \rangle$ is a function of the "bare" input parameters g, L and M

$$\langle F_{\mathrm{LAT}} \rangle = \langle F_{\mathrm{LAT}}(g, L, M) \rangle = \langle F(g) \rangle + \mathcal{O}(L^{-1}) + \mathcal{O}\left(e^{-LM}\right). \tag{5.1.4}$$

For fixed g one chooses a fixed LM, large enough to keep finite volume effects $\mathcal{O}\left(e^{-LM}\right)$ small. For each finite value L there will be a difference of $\langle F_{\mathrm{LAT}} \rangle$ and its continuum equivalent by means of lattice artefacts $\mathcal{O}(L^{-1})$. The continuum limit $\langle F(g) \rangle$ is obtained via an extrapolation to infinite L.

5.2 Simulation parameters

As mentioned we employ different lattice sizes varying between $L = 8$ and $L = 32$. In the HMC simulation the MD equations of motion are evaluated along a fictitious MC time τ. For one trajectory we utilize a MC time of $\tau = 0.5$ with by default 100 integrator steps and therefore $\epsilon = \delta\tau = 0.005$. For the fractional powers of the fermion matrix we use a rational approximation (4.3.3) of degree $P = 15$ with the two sets of parameters stated in Table 5.2.1. We checked for a subset of the configurations that is accuracy is always better than 10^{-3} for $\xi^\dagger \left(\mathcal{O}_{\mathrm{F}}^\dagger \mathcal{O}_{\mathrm{F}}\right)^{-\frac{1}{4}} \xi$.

ρ	i	α_i	β_i
	0	3.2148873149863206	-
	1	$-2.2977600408751347 \cdot 10^{-9}$	$5.5367335615411457 \cdot 10^{-8}$
	2	$-1.6898103706901084 \cdot 10^{-8}$	$4.6910257304582898 \cdot 10^{-7}$
	3	$-1.1099658368596436 \cdot 10^{-7}$	$2.6768223190551614 \cdot 10^{-6}$
	4	$-7.2162146587729939 \cdot 10^{-7}$	$1.4319657256375662 \cdot 10^{-5}$
	5	$-4.6841070484595924 \cdot 10^{-6}$	$7.5694473187855338 \cdot 10^{-5}$
	6	$-3.0396303865820389 \cdot 10^{-5}$	$3.9922490005559548 \cdot 10^{-4}$
1/8	7	$-1.9723870959636086 \cdot 10^{-4}$	$2.1046795395127538 \cdot 10^{-3}$
	8	$-1.2798599250624023 \cdot 10^{-3}$	$1.1094832053548640 \cdot 10^{-2}$
	9	$-8.3051856063983548 \cdot 10^{-3}$	$5.8486687698920667 \cdot 10^{-2}$
	10	$-5.3904877281192094 \cdot 10^{-2}$	$3.0834388405073770 \cdot 10^{-1}$
	11	$-3.5026088217184553 \cdot 10^{-1}$	1.6264534005778293
	12	-2.2893521967679966	8.6030459456576764
	13	$-1.5436668340425719 \cdot 10$	$4.6179583183155444 \cdot 10$
	14	$-1.2297861076048798 \cdot 10^{2}$	$2.6854965277696181 \cdot 10^{2}$
	15	$-2.6252652966414048 \cdot 10^{3}$	$2.6004158696112045 \cdot 10^{3}$
	0	$9.5797060554725838 \cdot 10^{-2}$	-
	1	$1.7701746700099842 \cdot 10^{-6}$	$3.1085594175442315 \cdot 10^{-8}$
	2	$5.8705983656937455 \cdot 10^{-6}$	$3.2994455960441383 \cdot 10^{-7}$
	3	$1.9961158693570120 \cdot 10^{-5}$	$1.9424842756552213 \cdot 10^{-6}$
	4	$6.9125367600088173 \cdot 10^{-5}$	$1.0453359626231250 \cdot 10^{-5}$
	5	$2.4032965323696816 \cdot 10^{-4}$	$5.5337819905761986 \cdot 10^{-5}$
	6	$8.3620125835371663 \cdot 10^{-4}$	$2.9204178440857227 \cdot 10^{-4}$
-1/4	7	$2.9099006745502945 \cdot 10^{-3}$	$1.5403300046437174 \cdot 10^{-3}$
	8	$1.0126504714418652 \cdot 10^{-2}$	$8.1233558140562465 \cdot 10^{-3}$
	9	$3.5241454044660878 \cdot 10^{-2}$	$4.2840454273820550 \cdot 10^{-2}$
	10	$1.2266034741624667 \cdot 10^{-1}$	$2.2594500626442715 \cdot 10^{-1}$
	11	$4.2721681852328125 \cdot 10^{-1}$	1.1921171782283737
	12	1.4932820692676758	6.3026182343759860
	13	5.3188766358452595	$3.3683411978650057 \cdot 10$
	14	$2.0944763089672641 \cdot 10^{1}$	$1.9083658214156412 \cdot 10^{2}$
	15	$1.4525770103354523 \cdot 10^{2}$	$1.5386784635765257 \cdot 10^{3}$

Table 5.2.1 Two sets of coefficients used for the rational approximation (4.3.3) sufficient for the exponents $\rho = 1/8$ and $\rho = -1/4$, respectively.

Appendix

A Grassmann numbers

A.1 Grassmann algebra

When we start considering a QFT including fermions, we have to conclude that our canonical quantisation rules for bosons no longer apply. Instead of a commutation relation

$$[\phi(x), \Pi(y)] = i\hbar\delta(x-y) \tag{A.1.1}$$

for bosonic fields, one has to introduce anticommutation relations for fermionic ones [26]

$$\{\psi(x), \pi(y)\} = i\hbar\delta(x-y), \tag{A.1.2}$$

which in the classical limit $\hbar \to 0$ is leading to objects that behave like anticommuting numbers

$$\psi\pi = -\pi\psi, \tag{A.1.3}$$

which seems rather strange at first. But the concept of anticommuting numbers, so called Grassmann variables, has proved quite useful in the path integral framework to represent the algebra of fermionic position and momentum observables as operators on a space of functions. In the following we want to define these objects and study their properties.

We can identify Grassmann numbers with elements of the exterior algebra $\Lambda^1(V)$ over a vector space V over a field K. According to the dimension of V the algebra has a finite collection of generators $\xi_1, \ldots, \xi_N$ with $N = \dim V \geq 1$ or infinitely many, if the vector space is infinite dimensional. With the exterior product there exists an associative connection on the algebra, which is linear in scalar multiplication and satisfies

$$\xi_i \wedge \xi_i = 0. \tag{A.1.4}$$

Thereby follows the demanded anticommutativity for the fermionic Grassmann variables

$$\xi_i \wedge \xi_j = -\xi_j \wedge \xi_i. \tag{A.1.5}$$

In general we can write the exterior algebra as a direct sum of subalgebras

$$\Lambda(V) = \bigoplus_{m=0}^{N} \Lambda^m(V), \tag{A.1.6}$$

where $\Lambda^m(V)$ is the quotient algebra of the tensor algebra $T^m(V)$ and the two-sided ideal $I^m(V)$ and $\Lambda^0(V) = K$. For an $a \in \Lambda^k(V)$ and $b \in \Lambda^l(V)$ we have a graded commutative exterior product

$$a \wedge b = (-1)^{kl} b \wedge a. \tag{A.1.7}$$

Therefore if we have an $a = \xi_i \wedge \xi_j$ and $b = \xi_m \wedge \xi_n$, then we get

$$a \wedge b = b \wedge a \tag{A.1.8}$$

and a and b behave like bosonic quantities. The highest alternating tensor one can create is

$$\xi_1 \wedge \xi_2 \wedge \ldots \wedge \xi_N \in \Lambda^N(V), \tag{A.1.9}$$

and with (A.1.4) it applies for all higher tensor spaces that $\Lambda^k(V) = 0,\ \forall\ k > N$. From now on we want to abbreviate the wedge notation simply by

$$\xi_i \xi_j \equiv \xi_i \wedge \xi_j. \tag{A.1.10}$$

So any analytic function of some real quantities $x_i \in \mathbb{R}$ and Grassmannian generators $\xi_j \in \Lambda(V)$ can be represented by finitely many terms

$$f(x_1, \ldots, x_n, \xi_1, \ldots, \xi_N) = f_0 + f_1\, \xi_1 + \ldots + f_{12}\, \xi_1 \xi_2 + \ldots + f_{1\ldots N}\, \xi_1 \cdots \xi_N, \tag{A.1.11}$$

where the coefficients are functions of the real quantities. In scope of this thesis we have to deal with vectors of four complex Grassmann variables and adapt our notation to the one used in [15]

$$\eta_i = \frac{1}{\sqrt{2}} \left(\xi_i^{\mathrm{R}} + i\, \xi_i^{\mathrm{I}} \right), \qquad \text{with} \quad \xi_i^{\mathrm{R}}, \xi_i^{\mathrm{I}} \in \Lambda^1(V), \quad i = (1, \ldots, 4). \tag{A.1.12}$$

We now define the Grassmann variables with an upper index as the complex conjugate of the ones with lower index $\eta^i \equiv (\eta_i)^\dagger = (\eta_i)^*$. Complex conjugation of two real Grassmann numbers is defined to include a change of position

$$(\xi_1 \xi_2)^* \equiv \xi_2^* \xi_1^* = -\xi_1 \xi_2. \tag{A.1.13}$$

They therefore behave like a formally purely imaginary quantity, whereas

$$(i \xi_1 \xi_2)^* = i \xi_1 \xi_2 \tag{A.1.14}$$

behaves like a formally real quantity.

A.2 Grassmann analysis

Now we want to see how we can differentiate and integrate Grassmann variables. We define the derivative to be

$$\frac{\partial \xi_m}{\partial \xi_n} \equiv \delta_{mn}. \tag{A.2.1}$$

Following [26] and [27] we define the product rule to satisfy

$$\frac{\partial}{\partial\xi_n}\left(\xi_{m_1}\xi_{m_2}\cdots\xi_{m_r}\right) \equiv \delta_{m_1 n}\,\xi_{m_2}\cdots\xi_{m_r} - \delta_{m_2 n}\,\xi_{m_1}\xi_{m_3}\cdots\xi_{m_r} + \cdots + (-1)^{r-1}\delta_{m_r n}\,\xi_{m_1}\cdots\xi_{m_r}. \tag{A.2.2}$$

The tangent vectors are also elements of the exterior algebra and satisfy the same anticommutation rules

$$\frac{\partial}{\partial\xi_i}\frac{\partial}{\partial\xi_j} = -\frac{\partial}{\partial\xi_j}\frac{\partial}{\partial\xi_i}. \tag{A.2.3}$$

So if we perform a coordinate transformation $\xi_i = M_{ij}\,\theta_j$, an n-form is transforming according to the alternating properties of forms like

$$\frac{\partial}{\partial\xi_1}\cdots\frac{\partial}{\partial\xi_n} = \det\left(M^{-1}\right)\frac{\partial}{\partial\theta_1}\cdots\frac{\partial}{\partial\theta_n}, \tag{A.2.4}$$

where the matrix M is associated with the Jacobian

$$M_{ij} = \frac{\partial\xi_i}{\partial\theta_j}. \tag{A.2.5}$$

For an integral $\mathcal{I}[f]$ of a function $f(\xi)$ it holds true that

$$\frac{\partial}{\partial\xi}\mathcal{I}[f] = 0, \tag{A.2.6}$$

since the integral is independent of the integration variable. With (A.1.4) it is also true that

$$\frac{\partial}{\partial\xi}\frac{\partial}{\partial\xi} = 0 \tag{A.2.7}$$

and therefore one can identify the integration on Grassmann numbers with the differentiation up to some normalization constant C

$$\mathcal{I}[f] = \int \mathrm{d}\xi\; f(\xi) = C\frac{\partial}{\partial\xi}f(\xi). \tag{A.2.8}$$

So we end up with the following integration rules, if we define $C \equiv 1$:

$$\int \mathrm{d}\xi\;\xi = \frac{\partial}{\partial\xi}\xi = 1, \qquad \int \mathrm{d}\xi\;1 = \frac{\partial}{\partial\xi}1 = 0. \tag{A.2.9}$$

We now want to perform an integration over the complex Grassmann variables η and $\eta^\dagger$. Therefore we want to investigate an integration over the function

$$e^{-a\eta\eta^\dagger}. \tag{A.2.10}$$

With

$$\eta\eta^\dagger = \frac{1}{2}\left(\xi_\mathrm{R} + i\,\xi_\mathrm{I}\right)\left(\xi_\mathrm{R} - i\,\xi_\mathrm{I}\right) = -i\,\xi_\mathrm{R}\xi_\mathrm{I} \tag{A.2.11}$$

and (A.2.4) we can transform the integral using that the determinant of the JACOBIAN is $\det J = i$ and find

$$\begin{aligned}\int \mathrm{d}\eta \mathrm{d}\eta^\dagger \; e^{-a\eta\eta^\dagger} &= i \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; e^{ia\xi_\mathrm{R}\xi_\mathrm{I}} \\ &= i \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; (1 + i\, a\xi_\mathrm{R}\xi_\mathrm{I}) \\ &= a \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; \xi_\mathrm{I}\xi_\mathrm{R} = a\end{aligned} \tag{A.2.12}$$

We get the same result by integrating over two real GRASSMANN variables ξ_1 and ξ_2

$$\int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \; e^{-a\xi_1\xi_2} = a. \tag{A.2.13}$$

By rewriting it with help of the antisymmetric matrix

$$A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix} \tag{A.2.14}$$

we get

$$\int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \; e^{-\frac{1}{2}\xi_i A_{ij} \xi_j} = \mathrm{Pf}\,(A)\,, \tag{A.2.15}$$

where $\mathrm{Pf}\,(A)$ is the PFAFFIAN of A, which is defined by the factorisation of the determinant in the following way

$$\mathrm{Pf}\,(A)^2 = \det(A) \tag{A.2.16}$$

This relation holds true for an even number of arbitrary many GRASSMANN generators. Its is therefore possible to integrate out GRASSMANN variables and be left with calculating a determinant or PFAFFIAN, which comes in quite essential when dealing with GRASSMANN integrals numerically.

A.3 Hubbard-Stratonovich transformation

We have now seen how to deal with bilinear exponentials. But in many cases one also has to deal with higher forms than bilinears. In principle one can expand any function into finitely many terms, like we have seen earlier, and then perform the integration rules, which is but rather ugly and proved not very efficient in numerical simulations. But there is a method to transform an exponential with 4-forms into one with bilinears, by performing an integration over additional bosonic auxiliary fields. This is called a HUBBARD-STRATONOVICH transformation. Assuming that we have a finite number of complex GRASSMANN variables η_i, we can see that the object $\eta^2 \equiv \eta^i \eta_i$ transforms like a formally real quantity

$$\left(\eta^i \eta_i\right)^* = (\eta_i)^* \left(\eta^i\right)^* = \eta^i \eta_i. \tag{A.3.1}$$

Therefore $(\eta^2)^2$ is a formally positive real value and we can apply the identity

$$e^{\frac{(\eta^2)^2}{4a}} = \sqrt{\frac{a}{\pi}} \int \mathrm{d}\phi \, e^{-a\phi^2+\eta^2\phi}, \tag{A.3.2}$$

which one can proof simply by square addition and performing a GAUSSIAN integral. If we see this identity in the context of the path integral framework, we can say, that a new bosonic auxiliary field ϕ is introduced for the specific space time point, where the integration took place. Since we can do this transformation at every space time point, this leads to a whole path integral over ϕ. Now we also have to be aware of what happens if the exponent on the left side of (A.3.2) is negative

$$e^{-\frac{(\eta^2)^2}{4a}} = e^{\frac{(i\eta^2)^2}{4a}} = \sqrt{\frac{a}{\pi}} \int \mathrm{d}\phi \, e^{-a\phi^2+i\eta^2\phi}. \tag{A.3.3}$$

We can see that this introduces an imaginary term in the exponent and therefore a high oscillatory function in the integral. Analytically this term would not bother us, but since we want to perform a numerical calculation something like this often results into a numerical sign problem, discussed in section 2.3.4.

B $AdS_5 \times S^5$ spacetime

The $AdS_5 \times S^5$ space is in the central focus of the gauge/gravity duality and should be concerned more deeply. It is a direct product of five dimensional Anti-de Sitter (AdS) space and a five dimensional compact sphere. Both are maximally symmetric spaces and therefore inherit the isometry groups $SO(2,4)$ in case of AdS_5 and respectively $SO(6)$ for S^5 [3]. This is an important fact for the AdS/CFT correspondence since the direct product of these groups has the same amount of degrees of freedom as the superconformal group $SO(2,4) \times SO(6) = SU(2,2|4)$ as the undelying symmetry group of $\mathcal{N} = 4$ super YANG-MILLS theory in four dimensional MINKOWSKI space.

B.1 AdS_5 space

Since the construction of a sphere is rather simple, we focus on the Anti-de Sitter space. AdS_5 is a hyperboloid with constant negative curvature, that can be embedded in six dimensional MINKOWSKI spacetime $X = (X^0, X^1, \ldots, X^5) \in \mathbb{R}^{4,2}$, with metric $\tilde{\eta} = \mathrm{diag}(-,+,+,+,+,-)$, so that

$$\mathrm{d}s^2 = -\left(\mathrm{d}X^0\right)^2 + \left(\mathrm{d}X^1\right)^2 + \cdots + \left(\mathrm{d}X^4\right)^2 - \left(\mathrm{d}X^5\right)^2 = \tilde{\eta}_{MN}\mathrm{d}X^M\mathrm{d}X^N, \tag{B.1.1}$$

where $M, N \in 0, \ldots, 5$. AdS_5 is then given by the hypersurface

$$\tilde{\eta}_{MN}X^M X^N = -\left(X^0\right)^2 + \left(X^1\right)^2 + \cdots + \left(X^4\right)^2 - \left(X^5\right)^2 = -R^2, \tag{B.1.2}$$

where R is the radius of curvature of the AdS_5 space, see also Figure B.1.1 for an embedding of AdS_2 in $\mathbb{R}^3$. For large X^M the hyperboloid approaches the light-cone of the MINKOWSKI space $\mathbb{R}^{4,2}$, given by

$$\tilde{\eta}_{MN}X^M X^N = 0. \tag{B.1.3}$$

We therefore can define the 'boundary' ∂AdS_5 of Anti-de Sitter space by the set of all lines on the light-cone (B.1.3) originating from $0 \in \mathbb{R}^{4,2}$. For a point $X \neq 0$ in AdS_5 close to the boundary and therefore satisfying (B.1.3) we can define (u, v) by

$$u = X^5 + X^4, \qquad v = X^5 - X^4, \tag{B.1.4}$$

so we can rewrite (B.1.3) as

$$uv = \eta_{\mu\nu}X^\mu X^\nu, \tag{B.1.5}$$

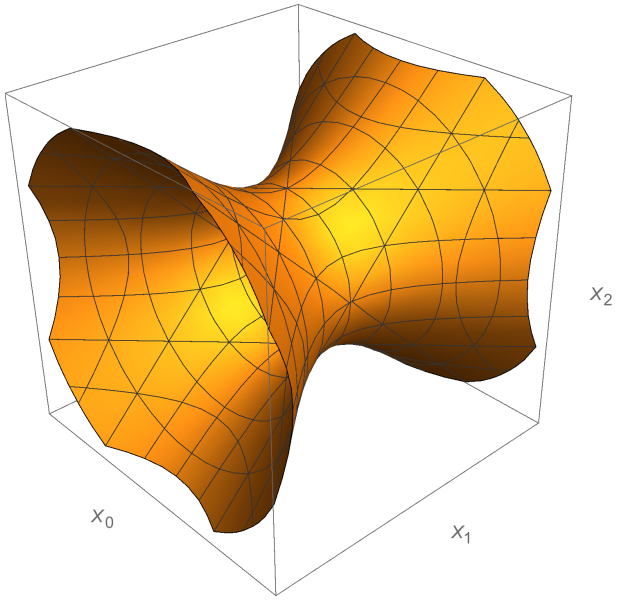

Figure B.1.1 Embedding of AdS_2 in $\mathbb{R}^3$ as a hypersurface given by the equation $-(X_0)^2 + (X_1)^2 - (X_3)^2 = -1$.

with $\mu, \nu \in 0, 1, 2, 3$ and $(\eta_{\mu\nu}) = \text{diag}(-, +, +, +)$. Whenever $v \neq 0$ we can rescale the coordinates to set $v = 1$ and solve for u. Therefore one is left with a four dimensional MINKOWSKI space $\mathbb{R}^{3,1}$. Points with $v = 0$ are "points at infinity" added to four dimensional MINKOWSKI space. This makes ∂AdS_5 a conformal compactification of four dimensional MINKOWSKI space. According to Maldacena [12] the correspondence between a $\mathcal{N} = 4$ theory on $\mathbb{R}^{3,1}$ and Type IIB on $AdS_5 \times S^5$ therefore expresses a string theory on $AdS_5 \times S^5$ in terms of a theory on the boundary and thus is referred to as "holographic" [28].

B.2 Poincaré patch

Let us now introduce a parametrisation of the hyperboloid (B.1.2) by the following coordinates $x^\mu \in \mathbb{R}$, for $\mu \in 0, 1, 2, 3$ and $z \in \mathbb{R}_+$. The parametrisation in these coordinates is given by (see e.g. [3, 29])

$$\begin{aligned} X^0 &= \frac{z}{2}\left(1 + \frac{1}{z^2}\left(x_\mu x^\mu + R^2\right)\right), \\ X^i &= \frac{R}{z}x^i, \quad i \in 1, 2, 3, \\ X^4 &= \frac{z}{2}\left(1 + \frac{1}{z^2}\left(x_\mu x^\mu - R^2\right)\right), \\ X^5 &= \frac{R}{z}x^0, \end{aligned} \tag{B.2.1}$$

with $x_\mu x^\mu = \eta_{\mu\nu} x^\mu x^\nu$ and $(\eta_{\mu\nu}) = \mathrm{diag}(-,+,+,+)$. These local coordinates are called POINCARÉ patch. The metric of AdS_5 in the POINCARÉ patch reads

$$\mathrm{d}s^2 = \frac{R^2}{z^2}\left(\mathrm{d}z^2 + \eta_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu\right). \tag{B.2.2}$$

For the whole $AdS_5 \times S^5$ space in POINCARÉ patch we find

$$\mathrm{d}s^2 = \frac{R^2}{z^2}\left(\mathrm{d}z^2 + \eta_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu\right) + \mathrm{d}u^I \mathrm{d}u^I, \tag{B.2.3}$$

where u^I $(I = 1, \ldots, 6)$ are coordinates on S^5 that satisfy $u^I u^I = R^2$. For $z \to 0$ we approach the boundary of $AdS_5 \times S^5$ and we can see from the metric that the contribution of the sphere becomes neglectable close to the boundary. If we include the infinite regime as $\partial(AdS_5 \times S^5)$ where $z = 0$ we can convince ourselves that the metric is conformally equivalent to 4d MINKOWSKI space.

C SO(6) matrices

The matrices ρ_{ij}^M appearing in the action (3.5.12) are the off-diagonal blocks of $SO(6)$ Dirac matrices γ^M in chiral representation[1]

$$\gamma^M \equiv \begin{pmatrix} 0 & \rho_M^\dagger \\ \rho^M & 0 \end{pmatrix} = \begin{pmatrix} 0 & (\rho^M)^{ij} \\ (\rho^M)_{ij} & 0 \end{pmatrix}. \tag{C.0.1}$$

The ρ_{ij}^M shall all skew symmetric and we define the ones with the upper indices to satisfy $(\rho^M)^{ij} \equiv (\rho_{ij}^M)^\dagger$. We can therefore state the following properties

$$\rho_{ij}^M = -\rho_{ji}^M, \qquad (\rho^M)^{ij} = -(\rho_{ij}^M)^*, \tag{C.0.2}$$

and we chose to use the following representation

$$\rho_{ij}^1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad \rho_{ij}^2 = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad \rho_{ij}^3 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$\rho_{ij}^4 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \rho_{ij}^5 = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \quad \rho_{ij}^6 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{C.0.3}$$

From the Clifford algebra of the Dirac matrices $\{\gamma^M, \gamma^N\} = 2\delta^{MN}\mathbb{1}_8$ we can derive the relation

$$(\rho^M)^{il}(\rho^N)_{lj} + (\rho^N)^{il}(\rho^M)_{lj} = 2\delta^{MN}\delta_j^i. \tag{C.0.4}$$

The generators of the $SO(6)$ can be built by

$$\left(\rho^{MN}\right)^i{}_j = \frac{1}{2}\left[\left(\rho^M\right)^{il}\left(\rho^N\right)_{lj} - \left(\rho^N\right)^{il}\left(\rho^M\right)_{lj}\right]. \tag{C.0.5}$$

Further relations and identities are

$$\left(\rho^{MN}\right)^i{}_j = \left(\rho^{MN}\right)_i^{*j}, \qquad \left(\rho^{MN}\right)^i{}_j = \left(\rho^{NM}\right)_j{}^i, \tag{C.0.6}$$

$$(\rho^M)^{im}(\rho^M)^{kn} = 2\epsilon^{imkn}, \qquad (\rho^M)^{im}(\rho^M)_{nj} = 2\left(\delta_j^i\delta_n^m - \delta_n^i\delta_j^m\right), \tag{C.0.7}$$

[1]The upper or lower placement of the index M on the block matrices has no meaning and is only changed for the purpose of readability.

$$\begin{aligned}
&\epsilon^{imkn}(\rho^M)_{mj}(\rho^L)_{nl} + \epsilon_{mjnl}(\rho^M)^{im}(\rho^L)^{kn} \qquad \text{(C.0.8)}\\
&= (\rho^{\{M})^{ik}(\rho^{L\}})^{jl} + \delta^k_j(\rho^L)^{im}(\rho^M)_{ml} + \delta^i_l(\rho^M)^{km}(\rho^L)_{mj}\\
&\quad + \delta^{ML}\left(-4\delta^i_l\delta^k_j + 2\delta^i_j\delta^k_l\right) \ ,\\
&-(\rho^{MN})^i{}_j(\rho^{ML})^k{}_l n_N n_L = -2(\rho^N)^{ik}(\rho^L)_{jl}n_N n_L - \delta^i_j\delta^k_l + 2\delta^i_l\delta^k_j \ . \qquad \text{(C.0.9)}
\end{aligned}$$

D Discrete Fourier transform

To perform a FOURIER transform on the lattice one needs to discretize it to deal with a finite sequence of N complex numbers $x_0, x_1, \ldots, x_{N-1}$. We define the discrete FOURIER transform X_k to be a vector in the base of roots of unit with components x_n as follows:

$$X_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} x_n \, e^{-2\pi i k n/N} \qquad k \in \mathbb{Z}. \tag{D.0.1}$$

We can limit the domain of k to a finite set, because the exponential is periodic in k. In the following we want to stick to the domain $k \in \left[-\frac{N}{2}+1, \ldots, \frac{N}{2}\right]$ and restrict us to even N. The inverse transform can be defined to be

$$x_n = \frac{1}{\sqrt{N}} \sum_{k=-N/2+1}^{N/2} X_k \, e^{2\pi i n k/N}, \tag{D.0.2}$$

where due to periodicy n is in the domain $[0, \ldots, N-1]$ like defined in the beginning. If we now insert (D.0.1) into (D.0.2) we end up with

$$x_n = \frac{1}{N} \sum_{k=-N/2+1}^{N/2} \left(\sum_{m=0}^{N-1} x_m e^{-2\pi i k m/N} \right) e^{2\pi i k n/N} \tag{D.0.3}$$

$$= \frac{1}{N} \sum_{k',m=0}^{N-1} x_m e^{2\pi i k'(n-m)/N}, \tag{D.0.4}$$

where we shifted the summation for k' to be in the same domain as m. This is now only equal to x_n if the following important relation holds true

$$\frac{1}{N} \sum_{k'=0}^{N-1} e^{2\pi i k'(n-m)/N} = \delta_{m,n}. \tag{D.0.5}$$

We can prove this easily. For $n = m$ this is trivial and for $n \neq m$ we make use of the geometric series

$$\sum_{k'=0}^{N-1} \left(e^{2\pi i c/N}\right)^{k'} = \frac{1 - e^{2\pi i c}}{1 - e^{2\pi i c/N}} = 0, \qquad |c| = |n-m| \in [1, \ldots, N-1]. \tag{D.0.6}$$

Now we want to apply the Fourier transform on the two dimensional lattice used throughout this thesis. We defined the lattice to be

$$\Lambda = \{n = (n_0, n_1)\,|n_0 = 1, \ldots, N_0\,;\; n_1 = 1, \ldots, N_1\}\,, \tag{D.0.7}$$

with $N_0 = T$ and $N_1 = L$. Therefore the total number of lattice points is given by

$$|\Lambda| \equiv TL. \tag{D.0.8}$$

Following [6] we now want to calculate the discrete Fourier transform $\tilde{f}(p)$ of a function $f(n)$. Here for $f(n)$ we impose toroidal boundary conditions

$$f(n + \hat{\imath} N_i) = e^{2\pi i \theta_i} f(n), \tag{D.0.9}$$

where $\hat{\imath}$ is a unit vector in the i-direction and $\theta_i = 0$ corresponds to periodic and $\theta_i = 1/2$ to anti-periodic boundary conditions. The discrete momentum space corresponding to these boundary conditions is given by

$$\widetilde{\Lambda} = \left\{p = (p_0, p_1)|\, p_i = \frac{2\pi}{aN_i}(k_i + \theta_i),\; k_i = -\frac{N_i}{2} + 1, \ldots, \frac{N_i}{2}\right\}. \tag{D.0.10}$$

With (D.0.1) and (D.0.2) we can express the the Fourier transform as

$$\tilde{f}(p) = \frac{1}{\sqrt{|\Lambda|}} \sum_{n \in \Lambda} f(n)\, e^{-ip \cdot na} \tag{D.0.11}$$

and for the inverse transform we find

$$f(n) = \frac{1}{\sqrt{|\Lambda|}} \sum_{p \in \widetilde{\Lambda}} \tilde{f}(p)\, e^{ip \cdot na}. \tag{D.0.12}$$

Here again the important relations hold

$$\frac{1}{|\Lambda|} \sum_{n \in \Lambda} \exp(i(p - p') \cdot na) = \delta(p - p') \equiv \delta_{k_0, k_0'} \delta_{k_1, k_1'} \tag{D.0.13}$$

$$\frac{1}{|\Lambda|} \sum_{p \in \widetilde{\Lambda}} \exp(ip \cdot (n - n')a) = \delta(n - n') \equiv \delta_{n_0, n_0'} \delta_{n_1, n_1'}. \tag{D.0.14}$$

E Discretized fermion matrix

Here we want to present the details leading to the discretized version (4.2.18) of the operator $\mathcal{O}_{\mathrm{F}}$. As emphasized in section 4.2.3 $\hat{\mathcal{O}}_{\mathrm{F}}$ is a $16V \times 16V$ matrix and we will continue to use the notation introduced there to write subdivided blocks of size $4V \times 4V$ to result in

$$\hat{\mathcal{O}}_{\mathrm{F}} = \begin{pmatrix} \hat{W}_+ & i\bar{\Delta}_0^{\mathrm{A}} & -i\left(\vec{\Delta}_1^{Z} + \frac{M}{2}\bar{Z}\right) & 0 \\ i\bar{\Delta}_0^{\mathrm{A}} & -\hat{W}_+^{\dagger} & 0 & -i\left(\vec{\Delta}_1^{Z^\dagger} + \frac{M}{2}\bar{Z}^\dagger\right) \\ i\left(\bar{\Delta}_1^{Z} - \frac{M}{2}\bar{Z}\right) & 0 & 2\left(\bar{\Delta}_1^{x} - \frac{M}{2}\bar{Z}^{x}\right) + \hat{W}_- & i\bar{\Delta}_0^{\mathrm{A}} - \hat{A}^{\mathrm{T}} \\ 0 & i\left(\bar{\Delta}_1^{Z^\dagger} - \frac{M}{2}\bar{Z}^\dagger\right) & i\bar{\Delta}_0^{\mathrm{A}} + \hat{A} & 2\left(\bar{\Delta}_1^{x^*} - \frac{M}{2}\bar{Z}^{x^*}\right) - \hat{W}_-^{\dagger} \end{pmatrix}. \tag{E.0.1}$$

First of all we should mention that the operator $\mathcal{O}_{\mathrm{F}}$ was of dimension $[a]^{-1}$ which has been absorbed into the fermionic fields to make them dimensionless. Therefore $\hat{\mathcal{O}}_{\mathrm{F}}$ is dimensionless as well, as are now all the bosonic and fermionic fields. Further $\hat{\mathcal{O}}_{\mathrm{F}}$ needs to be anti-symmetric which is why all the discretized derivatives need to be symmetric finite differences. As it is standard in lattice QCD to use anti-periodic boundary conditions in the temporal direction for the fermions [7], we will apply those here as well. For the spacial direction periodic boundary conditions shall be used. So starting from block $(1,2)$ we make the transition

$$i\partial_t \mathbb{1}_4 \longrightarrow i\bar{\Delta}_0^{\mathrm{A}}, \tag{E.0.2}$$

where we defined

$$\bar{\Delta}_0^{\mathrm{A}} \equiv \bar{\Delta}_0^{\mathrm{a}} \otimes \mathbb{1}_4, \qquad \bar{\Delta}_0^{\mathrm{a}} \equiv \left(\bar{\Delta}_0^{\mathrm{a}}\right)(l,p) = \frac{1}{2}\left(\delta^{\mathrm{a}}_{l_{+\hat{1}},p} - \delta^{\mathrm{a}}_{l_{-\hat{1}},p}\right). \tag{E.0.3}$$

Thereby the superscripts A, a refer to the property of the finite differences to respect anti-periodic boundary conditions, whereas p will refer to periodic ones. In the next block $(1,3)$ we have

$$-i\rho^M\left(\partial_s + \tfrac{m}{2}\right)\frac{z^M}{z^3} \longrightarrow -i\left(\vec{\Delta}_1^{Z} + \frac{M}{2}\bar{Z}\right). \tag{E.0.4}$$

Since z^M/z^3 is on the right, the derivative will also act on this term which we will have to consider in the discretization. Thus we introduce the definitions

$$Z \equiv Z_{ij}(l) = \rho_{ij}^M \frac{z^M(l)}{z^3(l)}, \qquad \bar{Z} \equiv \bar{Z}_{ij}(l,p) = \delta_{l,p} Z_{ij}(l), \tag{E.0.5}$$

$$\vec{\Delta}_1^{Z} \equiv \left(\vec{\Delta}_1^{Z}\right)_{ij}(l,p) = \frac{1}{2}\left[\delta^{\mathrm{p}}_{l_{+\hat{1}},p} Z_{ij}(l_{+\hat{1}}) - \delta^{\mathrm{p}}_{l_{-\hat{1}},p} Z_{ij}(l_{-\hat{1}})\right]. \tag{E.0.6}$$

The right arrow shall indicate that Z is on the right and respected by the derivative. In block $(3,1)$ we also have the same operator with arrow to the left which indicates that the derivative will not act on Z

$$\overleftarrow{\Delta}_1^Z \equiv \left(\overleftarrow{\Delta}_1^Z\right)_{ij}(l,p) = \frac{1}{2}\left[\delta^{\mathrm{p}}_{l_{+\hat{1}},p} - \delta^{\mathrm{p}}_{l_{-\hat{1}},p}\right] Z_{ij}(l). \tag{E.0.7}$$

In block $(3,3)$ we observe

$$2\frac{z^M}{z^4}\rho^M\left(\partial_s x - \tfrac{m}{2}x\right) \longrightarrow 2\left(\bar{\Delta}_1^x - \tfrac{M}{2}\bar{Z}^x\right), \tag{E.0.8}$$

where

$$\bar{Z}^x \equiv \bar{Z}^x_{ij}(l,p) = \delta_{l,p}\frac{Z_{ij}(l)}{z(l)}x(l), \tag{E.0.9}$$

$$\bar{\Delta}_1^x \equiv \left(\bar{\Delta}_1^x\right)_{ij}(l,p) = \frac{1}{2}\frac{Z_{ij}(l)}{z(l)}\left[\delta^{\mathrm{p}}_{l_{+\hat{1}},p}x(l_{+\hat{1}}) - \delta^{\mathrm{p}}_{l_{-\hat{1}},p}x(l_{-\hat{1}})\right]. \tag{E.0.10}$$

The discretized version of A is given by

$$\begin{aligned}\hat{A}_{ij}(l,p) =& -\delta_{ij}\delta_{lp}\frac{\sqrt{6}}{z(l)}\phi(l) + \delta_{lp}\frac{\widetilde{\phi}_{ij}(l)}{z(l)} \\ &+ i\frac{z^N(l)}{z(l)}\left(\rho^{MN}\right)_{ij}\left(\delta^{\mathrm{p}}_{l_{+\hat{1}},p}z^M(l_{+\hat{1}}) - \delta^{\mathrm{p}}_{l_{-\hat{1}},p}Z^M(l_{-\hat{1}})\right) \\ &+ \frac{1}{z^3(l)}\left(\rho^*_N\right)_{ik}\widetilde{\phi}_{sk}(l)\left(\rho^L\right)_{sj}z^N(l)z^L(l)\delta_{lp}.\end{aligned} \tag{E.0.11}$$

For the other variations of the finite differences one simply substitutes $Z^\dagger$ or x^* in the associated expressions to derive $\vec{\Delta}_1^{Z^\dagger}$ and $\bar{\Delta}_1^{x^*}$. Since $\hat{\mathcal{O}}_{\mathrm{F}}$ is anti-symmetric we need to meet the condition that $\vec{\Delta}_1^Z = -\left(\overleftarrow{\Delta}_1^Z\right)^{\mathrm{T}}$ which is easy to check. The same property is needed for the corresponding Wilson term. One can define it to consist of two parts $\hat{W}_\pm^{(1)}$ and $\hat{W}_\pm^{(2)}$ which obey $\hat{W}_\pm^{(1)} = -\left(\hat{W}_\pm^{(2)}\right)^{\mathrm{T}}$ and vice versa. The resulting Wilson term

$$\hat{W}_\pm = \frac{1}{2}\left(\hat{W}_\pm^{(1)} + \hat{W}_\pm^{(2)}\right) \tag{E.0.12}$$

is therefore skew-symmetric $\left(\hat{W}_\pm\right)^{\mathrm{T}} = -\hat{W}_\pm$ which is necessary since it is sitting on the diagonal blocks of $\hat{\mathcal{O}}_{\mathrm{F}}$. The single terms are constructed in the following way

$$\hat{W}_\pm^{(1)} = \frac{r}{2}\left[\vec{\Lambda}_0^Z \pm i\vec{\Lambda}_1^Z\right], \qquad \hat{W}_\pm^{(2)} = \frac{r}{2}\left[\overleftarrow{\Lambda}_0^Z \pm i\overleftarrow{\Lambda}_1^Z\right] \tag{E.0.13}$$

with

$$\begin{aligned}Z^z &\equiv Z^z_{ij}(l) = Z_{ij}(l)z(l) \\ \vec{\Lambda}_\alpha^Z &\equiv \left(\vec{\Lambda}_\alpha^Z\right)_{ij}(l,p) = 2\delta_{l,p}Z^z(l) - \delta_{l_{+\hat{\alpha}},p}Z^z(l_{+\hat{\alpha}}) - \delta_{l_{-\hat{\alpha}},p}Z^z(l_{-\hat{\alpha}}) \\ \overleftarrow{\Lambda}_\alpha^Z &\equiv \left(\overleftarrow{\Lambda}_\alpha^Z\right)_{ij}(l,p) = \left(2\delta_{l,p} - \delta_{l_{+\hat{\alpha}},p} - \delta_{l_{-\hat{\alpha}},p}\right)Z^z(l),\end{aligned} \tag{E.0.14}$$

where again the temporal finite differences need to respect anti-periodic and the spacial ones periodic boundary conditions. The actual implementation nonetheless is slightly different. There we constructed $\hat{W}_{\pm}$ to have its upper triangular matrix equal to $\hat{W}_{\pm}^{(1)}$ and the lower triangular matrix equal to $\hat{W}_{\pm}^{(2)}$ which in the end is leading to the same result.

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