1 Preliminaries

1.1 AdS/CFT correspondence

One of the most exciting discoveries in theoretical physics in the last decades was probably made by Maldacena in 1997 [1]. His famous conjecture , now widely known as AdS/CFT correspondence 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) 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 AdS/CFT correspondence is some sort of strong-weak coupling duality. It can relate a strong coupled field theory to its dual, a weakly curved gravity theory. The conjecture links two theories, that are very different in their physical interpretation but states, that they are mathematically equivalent.
The AdS part refers to a gravity theory on asymptotically Anti-de Sitter spacetime, in particular a Type IIB superstring theory on $AdS_5 \times S^5$. CFT stands for conformal field theory and refers in this sense to a $\mathcal{N} = 4$ Super Yang-Mills theory in $3 + 1$ dimensions. The correspondence states in its strongest from [2]

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

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

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.

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

$$g^2_{\mathrm{YM}} = 2\pi g_{\mathrm{s}} \quad \text{and} \quad 2\lambda \equiv 2g^2_{\mathrm{YM}} N = R^4/\alpha'^2 \,. \tag{1.1}$$

In the second equation we defined the 't Hooft coupling λ. String theory is yet best understood in the perturbative regime of weak coupling, why it is convenient to restrict the coupling on the string theory side to $g_{\mathrm{s}} \ll 1$, while keeping $R/\sqrt{\alpha'}$ constant. The AdS side therefore reduces

to classical string theory and no higher loop orders have to be taken into account. The quantity R^2/α' is kept constant. As well as g_s also the coupling on the CFT side needs to satisfy $g_\mathrm{YM} \ll 1$ while $g^2_\mathrm{YM}N$ is kept finite. We therefore have to take the large N limit $N \to \infty$ which is also known as the 'T HOOFT limit where the corresponding coupling λ is fixed. This corresponds to the planar limit of the gauge theory. We are now left with λ as the free parameter of the theory. In the so called weak form of AdS/CFT one refers to the limit of large λ and therefore $\alpha/R^2 \to 0$. This results in large curvature R and vanishing string length l_s which gives rise to the point particle limit of Type IIB superstring theory in form of Type IIB supergravity. So for large λ one is in the perturbative regime of string theory, whereas the gauge theory side is perturbatively accessible for $\lambda \ll 1$. We want to investigate the AdS/CFT correspondence numerically from the string theory side and therefore know solutions for large λ from perturbation theory. Now we can make use of the previously stated relation by going to smaller couplings where we leave the perturbative regime of string theory but enter the selfsame for the gauge theory side. This means that when we do numerical simulations for small couplings in string theory, then we still might be able to compare these results with predicted solutions of the perturbative regime of gauge theory.

1.2 Wilson loops

An important class of observables in gauge theories are non-local gauge invariant operators called WILSON loops. These operator 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 function from the WILSON loop. Now AdS/CFT correspondence tells us, that a certain minimal surface of a string world sheet corresponds to that same 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

$$W[\mathcal{C}] = \frac{1}{N}\mathrm{Tr}\left(\mathcal{P}\exp\left[i\oint_{\mathcal{C}} \mathrm{d}x^\mu A_\mu\right]\right). \tag{1.2}$$

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

$$i\oint_{\mathcal{C}} \mathrm{d}x^\mu A_\mu = i\int_0^1 \mathrm{d}s \frac{\mathrm{d}x^\mu}{\mathrm{d}s} A_\mu\left(x\left(s\right)\right). \tag{1.3}$$

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

$$\mathcal{P}\left(A\left(x\left(s_1\right)\right)A\left(x\left(s_2\right)\right)\right) = \begin{cases} A\left(x\left(s_1\right)\right)A\left(x\left(s_2\right)\right) & \text{for } s_1 > s_2, \\ A\left(x\left(s_2\right)\right)A\left(x\left(s_1\right)\right) & \text{for } s_2 > s_1. \end{cases} \tag{1.4}$$

1.3 Wilson loops in $\mathcal{N}=4$ Super Yang-Mills theory

Since the action of four-dimensional $\mathcal{N}=4$ SYM can be derived via dimensional reduction from $\mathcal{N}=1$ SYM in ten dimensions [3] one can construct a WILSON loop 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, which was proposed in [4], can be written as

$$\mathcal{W}[\mathcal{C}] = \frac{1}{N}\mathrm{Tr}\mathcal{P}\exp\left(\int_{\mathcal{C}} \mathrm{d}s\left(iA_\mu(x)\dot{x}^\mu + |\dot{x}|\phi_I(x)n^I\right)\right). \tag{1.5}$$

Here $I = 1,\ldots,6$ and n^I might be considered coordinates in S^5, which satisfy $\delta_{IK}n^I n^K = 1$. 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 [4]. Thus the expectation value of the MALDACENA-WILSON loop operator is given by a string partition function

$$\langle\mathcal{W}[\mathcal{C}]\rangle = Z_{\text{string}}[\mathcal{C}], \tag{1.6}$$

which is a path integral obeying sufficient boundary conditions

$$Z_{\text{string}}[\mathcal{C}] = \int\limits_{\partial X^\mu = \mathcal{C}} \mathcal{D}X^M\,\mathcal{D}h_{\alpha\beta}\,\exp\left(-S_{\text{string}}\left(X,h\right)\right). \tag{1.7}$$

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 $(\tau,\sigma)\in\Sigma$ and 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 (1.7) needs to meet the following boundary conditions

$$X^\mu|_{\partial\Sigma} = x^\mu(s)\,, \quad \left.\frac{\widetilde{X}^I}{|\widetilde{X}^I|}\right|_{\partial\Sigma} = n^I(s)\,, \quad \left.|\widetilde{X}^I|\right|_{\partial\Sigma} = 0\,, \tag{1.8}$$

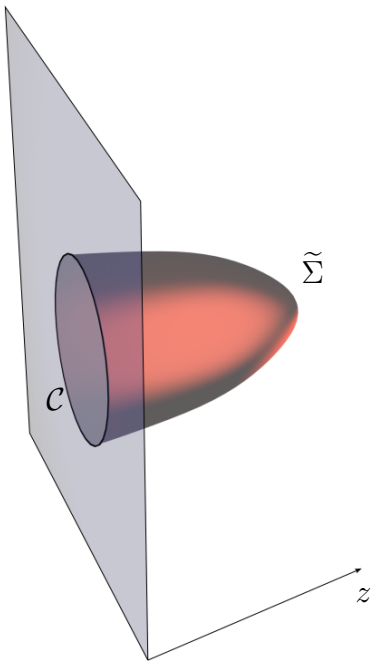

Figure 1.1 The embedding of the string worldsheet $\widetilde{\Sigma}$ in $AdS_5 \times S^5$ is bounded by the contour $\mathcal{C}$ as z approaches zero.

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 1.1. In the large 'T HOOFT coupling limit (1.7) can be evaluated with a saddle point approximation and results in the exponential of a minimal surface $\mathcal{A}_{\text{min}}(\mathcal{C})$ bounded by $\mathcal{C}$

$$\langle \mathcal{W}[\mathcal{C}] \rangle \simeq \exp\left(\frac{\sqrt{\lambda}}{2\pi} \mathcal{A}_{\text{min}}(\mathcal{C}) \right) . \tag{1.9}$$

1.4 Cusp anomalous dimension

To approach AdS/CFT in a numerical study it is important to observe a quantity that is widely known in different ranges of the 'T HOOFT coupling λ, so it 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 $\mathcal{N} = 4$ SYM

$$\mathcal{O}_{\{\mu_1 \cdots \mu_S\}} = \text{Tr}\, \phi^I \nabla_{\{\mu_1} \cdots \nabla_{\mu_S\}} \phi^I \,, \tag{1.10}$$

where ϕ^I are again the scalar fields of SYM. The conformal dimension of such operators is $\Delta_S = S + 2 + \gamma_S(\lambda)$ with γ_S being the anomalous dimension and

[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.

$\gamma_S \sim \ln S$ for $S \to \infty$. In [5] it was proposed that this conformal dimension corresponds to the energy of macroscopic rotating strings in the picture of supergravity for large S

$$E \simeq S + \frac{\sqrt{g_{\rm s}N}}{\pi} \ln S, \quad (S \to \infty)\,. \tag{1.11}$$

In [6], 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

$$\langle \mathcal{W}[\mathcal{C}_{\rm cusp}] \rangle \sim e^{-\Gamma_{\rm cusp}(\lambda,\gamma) \ln \frac{L}{\epsilon}} \xrightarrow{\gamma \to \infty} e^{-f(\lambda)|\gamma| \ln \frac{L}{\epsilon}}, \tag{1.12}$$

where γ is a boost angle in MINKOWSKI signature and $\Gamma_{\rm cusp}(\gamma, \lambda)$ 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 is also known as scaling function from integrability. It is related to the anomalous dimension of twist two operators via [7]

$$\gamma_S(\lambda) \simeq -2 f(\lambda) \ln S, \quad (S \to \infty). \tag{1.13}$$

The correspondence (1.6) 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 $\mathcal{C}_{\rm cusp}$. The remarks in [7, 8] suggest that the factor $|\gamma| \ln(L/\epsilon)$ corresponds to the regulated area of a cusped string worldsheet and is thus related to the world volume of the string $V_2 = \int {\rm d}\tau {\rm d}\sigma$, leading to

$$\langle \mathcal{W}[\mathcal{C}_{\rm cusp}] \rangle = e^{-\frac{f(\lambda)}{2} \frac{V_2}{4}}. \tag{1.14}$$

Semiclassical calculations with such vacua allowed to compute the scaling function up to two loops at strong coupling (see e.g. [9])

$$f(g) = 4g - \frac{3 \ln 2}{\pi} - \frac{K}{4\pi^2 g} + \mathcal{O}(g^{-2}), \quad g \equiv \frac{\sqrt{\lambda}}{4\pi}, \tag{1.15}$$

where $K \approx 0.916$ is the CATALAN constant. As mentioned the scaling function is also known from integrability where it can be derived from the BES[2] equation for any finite values of g. So our main aim is to reproduce the scaling function in numerical simulations.

1.5 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

[2] BES stands for Beisert-Eden-Staudacher equation, which is an integral equation derived via a BETHE Ansatz in quantum integrability [10].

by a cusp. Therefore we chose to follow the approach presented in [9]. We hereby start from a GREEN-SCHWARZ type superstring in AdS light-cone gauge with fixed κ-symmetry, that was proposed in [11, 12]. This action contains terms quadratic and quartic in fermions and has a classical solution $X_{\rm cl}$ forming a null-cusp on the AdS boundary. Now one can consider fluctuations around this classical solution and use (1.6) and (1.7) to match the vacuum expectation value of a WILSON loop around a null-cusp which is related to the scaling function via (1.12)

$$\langle \mathcal{W}_{\rm cusp} \rangle = \int \mathcal{D}\delta X \, \mathcal{D}\delta \Psi \; e^{-S_{\rm cusp}[X_{\rm cl}+\delta X, \delta\Psi]} = e^{-\frac{f(\lambda)}{2}\frac{V_2}{4}}. \tag{1.16}$$

Hereby $S_{\rm cusp}$ refers to the action expanded around the null-cusp solution $X_{\rm cl}$ and $\Psi_{\rm cl} = 0$, 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 $S_{\rm cusp}$. We will be using the $AdS_5 \times S^5$ metric in the POINCARÉ patch ($\mu = 0, \ldots, 3;\ M = 1, \ldots, 6$)

$$\mathrm{d}s^2 = z^{-2}\left(\mathrm{d}x^\mu \mathrm{d}x_\mu + \mathrm{d}z^M \mathrm{d}z^M\right) = z^{-2}\left(\mathrm{d}x^\mu \mathrm{d}x_\mu + \mathrm{d}z^2\right) + \mathrm{d}u^M \mathrm{d}u^M, \tag{1.17}$$

$$x^\mu x_\mu = x^+ x^- + x^* x, \quad x^\pm = x^3 \pm x^0, \quad x = x^1 + i x^2, \tag{1.18}$$

$$z^M = z u^M, \quad u^M u^M = 1, \quad z = \left(z^M z^M\right)^{\frac{1}{2}} \equiv e^\phi. \tag{1.19}$$

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 (1.19). In this case AdS_5 and S^5 have the same constant curvature radius $R = 1$. Starting point is the action from [13], 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

$$\sqrt{-h} h^{\alpha\beta} = \mathrm{diag}(-z^2, z^{-2}) \tag{1.20}$$

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

$$x^+ = p^+ \tau \tag{1.21}$$

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

$$S = g \int \mathrm{d}\tau \int \mathrm{d}\sigma \, \mathcal{L}, \qquad g \equiv \frac{\sqrt{\lambda}}{4\pi}, \tag{1.22}$$

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

where we defined $\eta^2 \equiv \eta^i \eta_i$. The six 4×4 matrices ρ^M and their properties are stated in Appendix **insert section**. 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 $\tau \to -i\tau$, $p^+ \to ip^+$ and after setting $p^+ = 1$ we obtain the euclidean action

$$
\begin{aligned}
S_\mathrm{E} &= g \int \mathrm{d}\tau \int \mathrm{d}\sigma \, \mathcal{L}_\mathrm{E}, \qquad (1.23)\\
\mathcal{L}_\mathrm{E} &= \dot{x}^* \dot{x} + \left(\dot{z}^M + i z^{-2} z^N \eta_i \big(\rho^{MN}\big)^i{}_j \eta^j \right)^2 + i \left(\theta^i \dot{\theta}_i + \eta^i \dot{\eta}_i + \theta_i \dot{\theta}^i + \eta_i \dot{\eta}^i \right) \\
&\quad - z^{-2} \left(\eta^2\right)^2 + z^{-4} \left(x'^* x' + z'^M z'^M \right) \\
&\quad + 2i \Bigg[z^{-3} \eta^i \rho^M_{ij} z^M \left(\theta'^j - i z^{-1} \eta^j x' \right) + z^{-3} \eta_i \left(\rho^\dagger_M \right)^{ij} z^M \left(\theta'_j + i z^{-1} \eta_j x'^* \right) \Bigg],
\end{aligned}
$$

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

$$
x^+ = \tau, \quad x^- = -\frac{1}{2\sigma}, \quad x^1 = x^2 = 0, \quad z = \sqrt{-2x^+x^-} = \sqrt{\frac{\tau}{\sigma}}, \qquad (1.24)
$$
$$
\tau, \sigma \in (0, \infty).
$$

For $z \to 0$ we approach the AdS boundary and therefore the regime of $\mathcal{N} = 4$ SYM. The curve proceeding at the boundary can be parametrised by

$$
\begin{aligned}
\mathcal{C}_\mathrm{cusp} \quad : \quad (-\infty, \infty) \quad &\longrightarrow \quad \mathbb{R}^{4,1} \\
s \quad &\longrightarrow \quad x^1 = x^2 = 0, \qquad (1.25)\\
&\qquad\qquad x^+ = \begin{cases} -s & s < 0, \\ 0 & \text{else}, \end{cases} \\
&\qquad\qquad x^- = \begin{cases} s & s > 0, \\ 0 & \text{else}. \end{cases}
\end{aligned}
$$

To arrive at the form of (1.16) with a fluctuation action S_cusp, we need to expand S_E around the null-cusp background (1.24). We therefore choose the field fluctuations to be

$$
x = \sqrt{\frac{\tau}{\sigma}} \tilde{x}, \quad z^M = \sqrt{\frac{\tau}{\sigma}} \tilde{z}^M, \quad \theta_i = \frac{1}{\sqrt{\sigma}} \tilde{\theta}_i, \quad \eta_i = \frac{1}{\sqrt{\sigma}} \tilde{\eta}_i. \qquad (1.26)
$$

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

$$S_{\text{cusp}} = g \int \mathrm{d}t \int \mathrm{d}s \, \mathcal{L}_{\text{cusp}} \tag{1.27}$$

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

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.

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 also provides a natural attempt to regularization, which makes it also an interesting topic for theorists in the field of QCD.

2.1 Discretizing the Lattice

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. We therefore need to limit the amount of points that we consider to make calculations. Since all the target space coordinates[3] 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 [14] we define the two-dimensional lattice Λ to be

$$\Lambda = \{(n_0, n_1) \,|n_0 = 1, 2, \ldots, T \,;\; n_1 = 1, 2, \ldots, L\} \,. \tag{2.1}$$

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

$$(\tau, \sigma) = (an_0, an_1) \,. \tag{2.2}$$

And since the lattice spacing is overall constant we can abbreviatly refer to

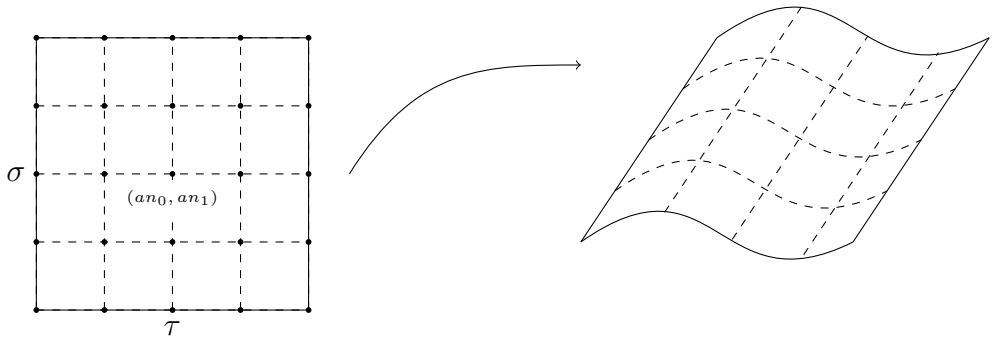

Figure 2.1 Mapping of the worldsheet grid into target space.

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

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

is introduced compared to the exact derivative, we examine the TAYLOR expansion of a real function $f(x)$ with a small offset ϵ

$$f(x \pm \epsilon) = f(x) \pm \epsilon f'(x) + \frac{\epsilon^2}{2} f''(x) \pm \frac{\epsilon^3}{6} f'''(x) + \dots . \tag{2.3}$$

Now we can define a forward derivative as the finite difference

$$\frac{f(x+\epsilon) - f(x)}{\epsilon} = f'(x) + \mathcal{O}(\epsilon) \tag{2.4}$$

and 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.

$$\frac{f(x-\epsilon) - f(x+\epsilon)}{2\epsilon} = f'(x) + \mathcal{O}(\epsilon^2). \tag{2.5}$$

It is more convenient to use the symmetric derivative, because the error introduced by the finite lattice spacing is therefore 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[4]

$$\partial_i \Phi(\sigma_j) = \widehat{\partial}_i \Phi(n) + \mathcal{O}(a^2) \equiv \frac{\Phi(n - \hat{\imath}) - \Phi(n + \hat{\imath})}{2a} + \mathcal{O}(a^2), \tag{2.6}$$

$$\text{with} \qquad \partial_i \Phi(\sigma_j) \equiv \frac{\partial \Phi(\sigma_j)}{\partial \sigma_i}, \qquad \sigma_i = (\tau, \sigma), \qquad i = 0, 1 \tag{2.7}$$

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

$$\int \mathrm{d}\tau \mathrm{d}\sigma \longrightarrow a^2 \sum_{n \in \Lambda}. \tag{2.8}$$

For a better visualization it is more convenient to use an abbreviated vector and matrix notation. In the following we will denote $\phi \equiv \phi_i(n)$ as a vector of fields which do each depend on the lattice coordinates n. The same is true for a matrix $M \equiv M_{ij}(m, n)$. A shorter expression of a matrix vector product is therefore

$$\phi^T M \psi \equiv \sum_{i,j} \sum_{m,n \in \Lambda} \phi_i(m) M_{ij}(m, n) \psi_j(n)\,. \tag{2.9}$$

[4]With $\widehat{\partial}_i$ beeing the symmetric derivative in i-direction. We also define the forward and backward derivative respectively by

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

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 derivative and a backward derivative

$$\widehat{\partial}_i^2 \Phi(n) = \overleftarrow{\partial}_i \vec{\partial}_i \Phi(n) = \frac{\Phi(n+\hat{\imath}) - 2\Phi(n) + \Phi(n-\hat{\imath})}{a^2}. \tag{2.10}$$

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

$$\Phi(n)\widehat{\partial}_i^2 \Phi(n) = \sum_{m\in\Lambda} \Phi(n)\widehat{\partial}_i^2(n,m)\,\Phi(m), \tag{2.11}$$

where we use (2.10) to define

$$\widehat{\partial}_i^2(n,m) \equiv \frac{\delta_{m,n+\hat{\imath}} - 2\delta_{m,n} + \delta_{m,n-\hat{\imath}}}{a^2}. \tag{2.12}$$

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 FOURIER transorm, that has been discussed in the Appendix. 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 [14]

$$\begin{aligned}
\widetilde{\partial}_i^2(p,q) &= \frac{1}{|\Lambda|}\sum_{m,n\in\Lambda} \mathrm{e}^{-\mathrm{i}q\cdot na}\,\widehat{\partial}_i^2(n,m)\,\mathrm{e}^{\mathrm{i}p\cdot ma} \\
&= \frac{1}{|\Lambda|}\sum_{n\in\Lambda} \mathrm{e}^{-\mathrm{i}(q-p)\cdot na}\frac{1}{a^2}\left[\mathrm{e}^{\mathrm{i}p_i a} - 2 + \mathrm{e}^{-\mathrm{i}p_i a}\right] \\
&= \delta(p-q)\,\widetilde{\partial}_i^2(p),
\end{aligned} \tag{2.13}$$

where the FOURIER transform of the second derivative is defined by

$$\widetilde{\partial}_i^2(p) \equiv -\frac{4}{a^2}\sin^2\left(\frac{p_i a}{2}\right). \tag{2.14}$$

The euclidean KLEIN-GORDON operator $\widetilde{D}(p)$ in momentum space with particle mass m is therefore

$$\widetilde{D}(p) = m^2 + \sum_{i=0}^{1} \widetilde{\partial}_i^2(p). \tag{2.15}$$

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

$$\widetilde{D}^{-1}(p)\Big|_{m=0} = \frac{1}{-\frac{4}{a^2}\sum_{i=0}^{1}\sin^2\left(\frac{p_i a}{2}\right)} \xrightarrow{a\to 0} -\frac{1}{p^2}. \tag{2.16}$$

This is precisely what we expected for the euclidean propagator in the continuum. Since we have $p_i \in \left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$, 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 as 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. We can now 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 derivative

$$\widehat{\partial}_i(m, n) \equiv \frac{\delta_{m,n+\hat{\imath}} - \delta_{m,n-\hat{\imath}}}{2a} \tag{2.17}$$

and proceed with the Fourier transform

$$\widetilde{\partial}_i(p, q) = \frac{1}{|\Lambda|}\sum_{m,n\in\Lambda} \mathrm{e}^{-\mathrm{i}q\cdot na}\,\widehat{\partial}_i(n, m)\,\mathrm{e}^{\mathrm{i}p\cdot ma} \tag{2.18}$$

$$= \frac{1}{|\Lambda|}\sum_{n\in\Lambda} \mathrm{e}^{-\mathrm{i}(q-p)\cdot na}\left[\frac{\mathrm{e}^{\mathrm{i}p_i a} - \mathrm{e}^{-\mathrm{i}p_i a}}{2a}\right] \tag{2.19}$$

$$= \delta(p - q)\,\widetilde{\partial}_i(p), \tag{2.20}$$

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

$$\widetilde{\partial}_i(p) \equiv \frac{\mathrm{i}}{a}\sin(p_i a). \tag{2.21}$$

To construct an euclidean Dirac like operator in two dimensions we use the first two Pauli matrices[5]

$$\widetilde{D}_D(p) = m\mathbb{1} + \sum_{i=0}^{1}\gamma_i\,\widetilde{\partial}_i(p) = m\mathbb{1} + \frac{\mathrm{i}}{a}\sum_{i=0}^{1}\gamma_i\sin(p_i a) \tag{2.22}$$

[5]
$$\gamma_0 = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \gamma_1 = \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$$

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

$$\widetilde{D}_D^{-1}(p) = \frac{m\mathbb{1} - \frac{\mathrm{i}}{a}\sum_{i=0}^{1}\gamma_i \sin(p_i a)}{m^2 + a^{-2}\sum_{i=0}^{1}\sin^2(p_i a)}. \tag{2.23}$$

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

$$\widetilde{D}_D^{-1}(p)\Big|_{m=0} = \frac{-\frac{\mathrm{i}}{a}\sum_{i=0}^{1}\gamma_i \sin(p_i a)}{a^{-2}\sum_{i=0}^{1}\sin^2(p_i a)} \xrightarrow{a\to 0} \frac{-\mathrm{i}\sum_{i=0}^{1}\gamma_i p_i}{p^2}. \tag{2.24}$$

Here again the propagator has the correct naive continuum limit but this time we face another problem. Since again p_i is in the domain $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right]$, there occur three other non-physical poles within the sine function at $p = (0, \pi/a)$, $p = (\pi/a, 0)$ and $p = (\pi/a, \pi/a)$. It therefore seems in the numerical simulation 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 then introduced a possible solution. He suggested to subtract the discretized LAPLACE operator times half the lattice spacing [15], which is known as a WILSON term, that we can express in momentum space with the help of (2.14) and find[6]

$$W(p) \equiv -\mathbb{1}\frac{a}{2}\sum_{i=0}^{1}\widetilde{\partial}_i^2(p) = \mathbb{1}\frac{1}{a}\sum_{i=0}^{1}\left(1 - \cos(p_i a)\right). \tag{2.25}$$

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 $p_i = 0$ and gives therefore no contribution to the physical pole of the theory. If we now invert the new DIRAC-WILSON operator

$$\widetilde{D}_W(p) \equiv \widetilde{D}_D(p) + W(p), \tag{2.26}$$

we find the new massless momentum space propagator

$$\widetilde{D}_W^{-1}\Big|_{m=0} = \frac{\mathbb{1}\frac{1}{a}\sum_{i=0}^{1}\left(1 - \cos(p_i a)\right) - \frac{\mathrm{i}}{a}\sum_{i=0}^{1}\gamma_i \sin(p_i a)}{\left(\frac{1}{a}\sum_{i=0}^{1}\left(1 - \cos(p_i a)\right)\right)^2 + \frac{1}{a^2}\sum_{i=0}^{1}\sin^2(p_i a)}. \tag{2.27}$$

Here we can convince ourselves, that there are no more additional poles in the domain of p_i, since for the points where $p_i = \pi/a$ 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 therefore decouples from the theory.

[6] using the identity

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

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 [16]

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi \, O(\phi) \exp\left(-S\left[\phi\right]\right), \tag{2.28}$$

where S is the euclidean action dependant on the collection of fields ϕ and Z is the partition function

$$Z = \int \mathcal{D}\phi \, \exp\left(-S\left[\phi\right]\right). \tag{2.29}$$

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

$$\mathcal{D}\phi = \prod_{n \in \Lambda} \mathrm{d}\phi(n). \tag{2.30}$$

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 scope of this theses.

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

$$I = \int_{\Omega} f(x) \, \mathrm{d}x, \tag{2.31}$$

where $\Omega \subset \mathbb{R}^n$ is a compact integration domain. Then probability theory tells us [17], 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

$$I_N = V \frac{1}{N} \sum_{i=1}^{N} f(\overline{x}_i). \tag{2.32}$$

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 $\lim_{N\to\infty} I_N = I$. One can also write for the expectation value $\langle f \rangle$ of f, that

$$\langle f \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(\overline{x}_i) = \frac{\int_\Omega f(x)\,\mathrm{d}x}{\int_\Omega \mathrm{d}x}. \tag{2.33}$$

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

$$H(x,y) = \begin{cases} 1 & \text{if} \quad x^2 + y^2 \leq 1 \\ 0 & \text{else.} \end{cases} \tag{2.34}$$

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

$$\pi \approx \frac{4}{N} \sum_{i=1}^{N} H(\overline{x}_i). \tag{2.35}$$

This means that we can estimate the value of $\pi/4$ by counting the number of points lying within the circle (see figure 2.2) and dividing by the total number of points.

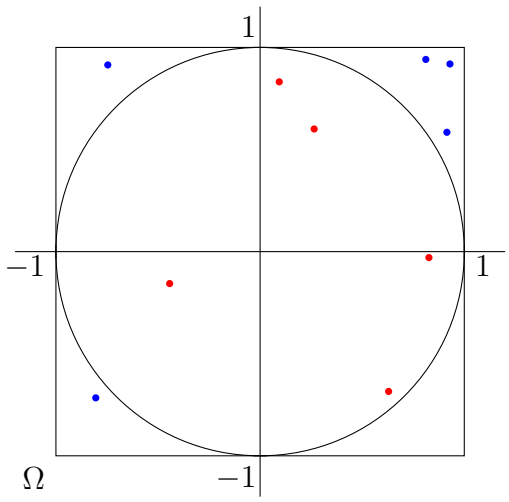

Figure 2.2 Graphic of random numbers uniform in Ω. $\pi/4$ can be estimated by the number of red points within the circle divided by total number of points.

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

$$\langle f \rangle_\rho \equiv \frac{\int_\Omega f(x)\rho(x)\,\mathrm{d}x}{\int_\Omega \rho(x)\,\mathrm{d}x} = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(\overline{x}_i). \tag{2.36}$$

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 (2.28) 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 [18]

$$\langle f \rangle_\rho = \int_a^b f(x)\rho(x)\,\mathrm{d}x\,, \quad \int_a^b \rho(x)\,\mathrm{d}x = 1. \tag{2.37}$$

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

$$P(x) = \int_a^x \rho(t)\,\mathrm{d}t. \tag{2.38}$$

If we perform the substitution

$$y(x) \equiv P(x), \quad \text{with} \quad \rho(x) = P'(x) = y'(x), \quad y \in [0,1], \tag{2.39}$$

we are left with

$$\langle f \rangle_\rho = \int_a^b f(x)y'(x)\,\mathrm{d}x = \int_0^1 f\left(x\left(y\right)\right)\mathrm{d}y, \tag{2.40}$$

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

$$\langle f \rangle_\rho = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(\overline{x}_i). \tag{2.41}$$

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 $P(\phi)$ [14]. The configurations in the chain can be numbered by an index, the so called Monte Carlo time

$$\phi_0 \to \phi_1 \to \ldots \to \phi_{N_{\text{th}}} \to \ldots \ . \tag{2.42}$$

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

$$0 \leq T(\phi'|\phi) \leq 1, \quad \sum_{\phi} T(\phi'|\phi) = 1. \tag{2.43}$$

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

$$\sum_{\phi} T(\phi'|\phi)P(\phi) = \sum_{\phi} T(\phi|\phi')P(\phi'). \tag{2.44}$$

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

$$T(\phi'|\phi)P(\phi) = T(\phi|\phi')P(\phi'). \tag{2.45}$$

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 chapter **INSERT SECTION**, 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 therefore write

$$\mathrm{Pf}\, M = (\det M)^{\frac{1}{2}} = \left(\det M M^\dagger\right)^{\frac{1}{4}}. \tag{2.46}$$

In general one could have to deal with an arbitrary fraction α in the exponent on the right side of (2.46). 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 η

$$\left(\det M M^\dagger\right)^\alpha = \frac{1}{\det\left(MM^\dagger\right)^{-\alpha}} \sim \int \mathcal{D}\eta\, \mathcal{D}\eta^\dagger\; e^{-\eta^\dagger (MM^\dagger)^{-\alpha}\eta}. \tag{2.47}$$

Since there is an invasion 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. One therefore 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 [19]. A more detailed explanation is presented in [14, 15] 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 ξ is generated from a GAUSSIAN distribution $P(\xi) \sim e^{-\xi^\dagger \xi}$ and we set $\eta = M\xi$. In the second phase a molecular dynamic evolution is used to update the bosonic fields while the pseudofermions are kept constant. We can therefore think of the effective action $S_{\mathrm{eff}}[\phi] = S_{\mathrm{B}}[\phi] + \eta^\dagger (MM^\dagger)^{-1}\eta$ 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

$$\langle O \rangle = \frac{\int \mathcal{D}\phi \mathcal{D}\eta \mathcal{D}\pi\; O(\phi)\, e^{-H[\phi,\pi]}}{\int \mathcal{D}\phi \mathcal{D}\eta \mathcal{D}\pi\; e^{-H[\phi,\pi]}}, \tag{2.48}$$

where we have introduced the HAMILTONIAN

$$H[\phi,\pi] = \frac{1}{2}\pi^2 + S_{\text{eff}}[\phi]\,, \quad \pi^2 = \sum_i \sum_{n\in\Lambda} \pi_i^2(n)\,. \tag{2.49}$$

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

$$\begin{aligned} \dot{\pi}_i &= -\frac{\partial H}{\partial \phi_i} = -\frac{\partial S_{\text{eff}}}{\partial \phi_i} \\ \dot{\phi}_i &= \frac{\partial H}{\partial \pi_i} = \pi_i \end{aligned} \tag{2.50}$$

A numerical implementation of (2.50) 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. Therefore, 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

$$\begin{aligned} \pi_i(\tfrac{\epsilon}{2}) &= \pi_i(0) - \frac{\partial S_{\text{eff}}(\phi(0))}{\partial \phi_i}\frac{\epsilon}{2}, \\ \phi_i(\epsilon) &= \phi_i(0) + \pi_i(\tfrac{\epsilon}{2})\epsilon\,. \end{aligned} \tag{2.51}$$

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

$$\begin{aligned} \pi_i\left(\left(j+\tfrac{1}{2}\right)\epsilon\right) &= \pi_i\left(\left(j-\tfrac{1}{2}\right)\epsilon\right) - \frac{\partial S_{\text{eff}}(\phi(j\epsilon))}{\partial \phi_i}\epsilon \\ \phi_i\left((j+1)\,\epsilon\right) &= \phi^i\left(j\epsilon\right) + \pi_i\left(\left(j+\tfrac{1}{2}\right)\epsilon\right)\epsilon\,. \end{aligned} \tag{2.52}$$

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

$$\pi_i(n\epsilon) = \pi_i\left(\left(n+\tfrac{1}{2}\right)\epsilon\right) - \frac{\partial S_{\text{eff}}(\phi(n\epsilon))}{\partial \phi_i}\frac{\epsilon}{2}\,. \tag{2.53}$$

With an additional METROPOLIS acceptance step $T_{\text{A}}(\phi',\pi'|\phi,\pi) = \min(1,\exp(H[\phi,\pi] - H[\phi',\pi'])$ the total transition probability to move from ϕ to ϕ' is given by

$$T(\phi'|\phi) = \int \mathcal{D}\pi'\mathcal{D}\pi\; T_{\text{A}}(\phi',\pi'|\phi,\pi) T_{\text{MD}}(\phi',\pi'|\phi,\pi) P_{\text{G}}(\pi)\,. \tag{2.54}$$

This has been proved to obey detailed balance in [19]. Concluding one can summarize the HMC algorithm in the following steps:

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

- **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

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

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

$$F_i[\phi] = \frac{\partial}{\partial\phi_i}\left[S_{\mathrm{B}}\left[\phi\right] + \eta^\dagger\left(MM^\dagger\right)^{-1}\eta\right]. \tag{2.55}$$

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

$$[\phi(x), \Pi(y)] = i\hbar\delta(x-y) \tag{A.1}$$

for bosonic fields, one has to introduce anticommutation relations for fermionic ones [20]

$$\{\psi(x), \pi(y)\} = i\hbar\delta(x-y), \tag{A.2}$$

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

$$\psi\pi = -\pi\psi, \tag{A.3}$$

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

$$\xi_i \wedge \xi_i = 0. \tag{A.4}$$

Thereby follows the demanded anticommutativity for the fermionic Grassmann variables

$$\xi_i \wedge \xi_j = -\xi_j \wedge \xi_i. \tag{A.5}$$

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

$$\Lambda(V) = \bigoplus_{m=0}^{N} \Lambda^m(V), \tag{A.6}$$

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

$$a \wedge b = (-1)^{kl} b \wedge a. \tag{A.7}$$

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

$$a \wedge b = b \wedge a \tag{A.8}$$

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

$$\xi_1 \wedge \xi_2 \wedge \ldots \wedge \xi_N \in \Lambda^N(V), \tag{A.9}$$

and with (A.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

$$\xi_i \xi_j \equiv \xi_i \wedge \xi_j. \tag{A.10}$$

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

$$f(x_1, \ldots, x_n, \xi_1, \ldots, \xi_N) = f_0 + f_1\, \xi_1 + \ldots + f_{12}\, \xi_1 \xi_2 + \ldots + f_{1\ldots N}\, \xi_1 \cdots \xi_N, \tag{A.11}$$

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 [9]

$$\eta_i = \frac{1}{\sqrt{2}} \left(\xi_i^{\mathrm{R}} + i\, \xi_i^{\mathrm{I}}\right), \qquad \text{with} \quad \xi_i^{\mathrm{R}}, \xi_i^{\mathrm{I}} \in \Lambda^1(V), \quad i = (1, \ldots, 4). \tag{A.12}$$

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

$$(\xi_1 \xi_2)^* \equiv \xi_2^* \xi_1^* = -\xi_1 \xi_2. \tag{A.13}$$

They therefore behave like a formally purely imaginary quantity, whereas

$$(i \xi_1 \xi_2)^* = i \xi_1 \xi_2 \tag{A.14}$$

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

$$\frac{\partial \xi_m}{\partial \xi_n} \equiv \delta_{mn}. \tag{A.15}$$

Following [20] and [21] we define the product rule to satisfy

$$\frac{\partial}{\partial\xi_n}\left(\xi_{m_1}\xi_{m_2}\cdots\xi_{m_r}\right) \equiv \delta_{m_1 n}\,\xi_{m_2}\cdots\xi_{m_r} - \delta_{m_2 n}\,\xi_{m_1}\xi_{m_3}\cdots\xi_{m_r} + \cdots + (-1)^{r-1}\delta_{m_r n}\,\xi_{m_1}\cdots\xi_{m_r}. \tag{A.16}$$

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

$$\frac{\partial}{\partial\xi_i}\frac{\partial}{\partial\xi_j} = -\frac{\partial}{\partial\xi_j}\frac{\partial}{\partial\xi_i}. \tag{A.17}$$

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

$$\frac{\partial}{\partial\xi_1}\cdots\frac{\partial}{\partial\xi_n} = \det\left(M^{-1}\right)\frac{\partial}{\partial\theta_1}\cdots\frac{\partial}{\partial\theta_n}, \tag{A.18}$$

where the matrix M is associated with the Jacobian

$$M_{ij} = \frac{\partial\xi_i}{\partial\theta_j}. \tag{A.19}$$

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

$$\frac{\partial}{\partial\xi}\mathcal{I}[f] = 0, \tag{A.20}$$

since the integral is independent of the integration variable. With (A.4) it is also true that

$$\frac{\partial}{\partial\xi}\frac{\partial}{\partial\xi} = 0 \tag{A.21}$$

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

$$\mathcal{I}[f] = \int \mathrm{d}\xi\; f(\xi) = C\frac{\partial}{\partial\xi}f(\xi). \tag{A.22}$$

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

$$\int \mathrm{d}\xi\;\xi = \frac{\partial}{\partial\xi}\xi = 1, \qquad \int \mathrm{d}\xi\;1 = \frac{\partial}{\partial\xi}1 = 0. \tag{A.23}$$

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

$$e^{-a\eta\eta^\dagger}. \tag{A.24}$$

With

$$\eta\eta^\dagger = \frac{1}{2}\left(\xi_\mathrm{R} + i\,\xi_\mathrm{I}\right)\left(\xi_\mathrm{R} - i\,\xi_\mathrm{I}\right) = -i\,\xi_\mathrm{R}\xi_\mathrm{I} \tag{A.25}$$

and (A.18) we can transform the integral using that the determinant of the Jacobian is $\det J = i$ and find

$$\begin{aligned}\int \mathrm{d}\eta \mathrm{d}\eta^\dagger \; e^{-a\eta\eta^\dagger} &= i \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; e^{ia\xi_\mathrm{R}\xi_\mathrm{I}} \\ &= i \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; (1 + i\, a\xi_\mathrm{R}\xi_\mathrm{I}) \\ &= a \int \mathrm{d}\xi_\mathrm{R} \mathrm{d}\xi_\mathrm{I} \; \xi_\mathrm{I}\xi_\mathrm{R} = a\end{aligned} \tag{A.26}$$

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

$$\int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \; e^{-a\xi_1\xi_2} = a. \tag{A.27}$$

By rewriting it with help of the antisymmetric matrix

$$A = \begin{pmatrix} 0 & a \\ -a & 0 \end{pmatrix} \tag{A.28}$$

we get

$$\int \mathrm{d}\xi_1 \mathrm{d}\xi_2 \; e^{-\frac{1}{2}\xi_i A_{ij} \xi_j} = \mathrm{Pf}\,(A)\,, \tag{A.29}$$

where $\mathrm{Pf}\,(A)$ is the Pfaffian of A, which is defined as the square root of the determinant of A. 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 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 field. 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

$$\left(\eta^i \eta_i\right)^* = (\eta_i)^* \left(\eta^i\right)^* = \eta^i \eta_i. \tag{A.30}$$

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

$$e^{\frac{(\eta^2)^2}{4a}} = \sqrt{\frac{a}{\pi}} \int \mathrm{d}\phi \; e^{-a\phi^2+\eta^2\phi}, \tag{A.31}$$

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.31) is negative

$$e^{-\frac{(\eta^2)^2}{4a}} = e^{\frac{(i\eta^2)^2}{4a}} = \sqrt{\frac{a}{\pi}} \int \mathrm{d}\phi \; e^{-a\phi^2+i\eta^2\phi}. \tag{A.32}$$

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 might turn out to be a problem. And in fact, like we will see later on, this will lead us to a so called sign problem.

B $\mathbf{AdS_5 \times S^5}$ 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 [2]. 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 $\mathbf{AdS_5}$ 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

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

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

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

where R is the radius of curvature of the AdS_5 space. For large X^M the hyperboloid approaches the light-cone of the MINKOWSKI space $\mathbb{R}^{4,2}$, given by

$$\tilde{\eta}_{MN} X^M X^N = 0. \tag{B.3}$$

We therefore can define the 'boundary' ∂AdS_5 of Anti-de Sitter space by the set of all lines on the light-cone (B.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.3) we can define (u, v) by

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

so we can rewrite (B.3) as

$$uv = \eta_{\mu\nu} X^\mu X^\nu, \tag{B.5}$$

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 [1] the correspondence between a $\mathcal{N} = 4$ theory an $\mathbb{R}^{3,1}$ 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" [22].

B.2 Poincaré patch

Let us now introduce a parametrisation of the hyperboloid (B.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

$$\begin{aligned} X^0 &= \frac{z}{2}\left(1 + \frac{1}{z^2}\left(x_\mu x^\mu + R^2\right)\right), \\ X^i &= \frac{R}{z} x^i, \quad i \in 1, 2, 3, \\ X^4 &= \frac{z}{2}\left(1 + \frac{1}{z^2}\left(x_\mu x^\mu - R^2\right)\right), \\ X^5 &= \frac{R}{z} x^0, \end{aligned} \tag{B.6}$$

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

$$\mathrm{d}s^2 = \frac{R^2}{z^2}\left(\mathrm{d}z^2 + \eta_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu\right). \tag{B.7}$$

C 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:

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

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

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

where due to periodicy n is in the domain $[0, \ldots, N-1]$ like defined in the beginning. If we now insert (C.1) into (C.2) we end up with

$$x_n = \frac{1}{N} \sum_{k=-N/2+1}^{N/2} \left(\sum_{m=0}^{N-1} x_m e^{-2\pi i k m/N} \right) e^{2\pi i k n/N} \tag{C.3}$$

$$= \frac{1}{N} \sum_{k',m=0}^{N-1} x_m e^{2\pi i k'(n-m)/N}, \tag{C.4}$$

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

$$\frac{1}{N} \sum_{k'=0}^{N-1} e^{2\pi i k'(n-m)/N} = \delta_{m,n}. \tag{C.5}$$

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

$$\sum_{k'=0}^{N-1} \left(e^{2\pi i c/N}\right)^{k'} = \frac{1 - e^{2\pi i c}}{1 - e^{2\pi i c/N}} = 0, \qquad |c| = |n-m| \in [1, \ldots, N-1]. \tag{C.6}$$

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

$$\Lambda = \{n = (n_0, n_1) \,|n_0 = 1, \ldots, N_0 \,;\; n_1 = 1, \ldots, N_1\}, \tag{C.7}$$

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

$$|\Lambda| \equiv TL. \tag{C.8}$$

Following [14] 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

$$f(n + \hat{\imath} N_i) = e^{2\pi i \theta_i} f(n), \tag{C.9}$$

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

$$\widetilde{\Lambda} = \left\{ p = (p_0, p_1) |\, p_i = \frac{2\pi}{a N_i}(k_i + \theta_i),\, k_i = -\frac{N_i}{2} + 1, \ldots, \frac{N_i}{2} \right\}. \tag{C.10}$$

With (C.1) and (C.2) we can express the the Fourier transform as

$$\tilde{f}(p) = \frac{1}{\sqrt{|\Lambda|}} \sum_{n \in \Lambda} f(n)\, e^{-ip \cdot na} \tag{C.11}$$

and for the inverse transform we find

$$f(n) = \frac{1}{\sqrt{|\Lambda|}} \sum_{p \in \widetilde{\Lambda}} \tilde{f}(p)\, e^{ip \cdot na}. \tag{C.12}$$

Here again the important relations hold

$$\frac{1}{|\Lambda|} \sum_{n \in \Lambda} \exp(i(p - p') \cdot na) = \delta(p - p') \equiv \delta_{k_0, k_0'} \delta_{k_1, k_1'} \tag{C.13}$$

$$\frac{1}{|\Lambda|} \sum_{p \in \widetilde{\Lambda}} \exp(ip \cdot (n - n')a) = \delta(n - n') \equiv \delta_{n_0, n_0'} \delta_{n_1, n_1'}. \tag{C.14}$$

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