Baryon mass and nuclear potential from Lattice QCD at strong coupling

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1 Introduction

In pursuit of a general framework for the description of elementary particle’s interactions, physicists in the first half of the last century expanded the formalism of quantum mechanics to that of quantum fields, combining the success of quantum mechanics with that of special relativity. The first successful quantum field theory resulting from that process was quantum electrodynamics (QED) which describes the interaction of charged spin-$\frac{1}{2}$ particles. The interaction is mediated by photons, the spin-1 gauge bosons of QED, and the underlying gauge group is $U(1)$. The predictions of QED were confirmed by experiments to very high precision. Subsequent effort to find a quantum field theory that describes all fundamental interactions of nature resulted in the Standard Model of elementary particle physics, which combines the strong, the weak and the electromagnetic interaction into one theory. The symmetry group of the Standard Model is denoted by $SU(3)_{\text{color}} \otimes SU(2)_{L} \otimes U(1)_{Y}$. Here $SU(N)$ and $U(N)$ denote the special unitary and unitary group of dimension $N$.

Of the interactions included in the Standard Model, the strong interaction, described by Quantum Chromodynamics (QCD), is of main interest in this thesis. Quantum Chromodynamics is a non-Abelian gauge theory and governs the interaction of quarks and gluons. Quarks are massive, color-charged spin-$\frac{1}{2}$ fermions, whereas gluons are massless spin-1 gauge bosons. In contrast to the photon of QED, gluons also carry a color charge and interact with each other. The symmetry group of QCD is $SU(3)_{\text{color}}$. Its non-Abelian nature introduces unique phenomena absent in other theories. The most important ones are asymptotic freedom and confinement. The former reflects the observation that the coupling $g_{s}$ weakens with decreasing distance \([1]\) and the latter states that only color-singlet states can be observed in nature.

To perform analytic calculations in quantum field theory, perturbative methods are usually applied. As a consequence of asymptotic freedom, perturbation theory converges well for short distances. The long range behavior, however, is intractable to perturbative treatments. To gain insight on the non-perturbative regime of QCD, K.G. Wilson proposed a discretization of the theory on a space-time lattice \([2]\). On the lattice, the path integral, an important mathematical tool in quantum field theory, is of finite dimension and can be evaluated by Monte-Carlo methods.

In this thesis, we want to investigate properties of nuclear matter such as the nucleon-nucleon potential $V_{NN}(r)$. Therefore, we have to perform Monte-Carlo simulations at non-zero baryon number. Such simulations suffer from the sign problem. To solve it, we use an approach based on the strong coupling limit $\beta \propto \frac{1}{g_{s}^{2}} \rightarrow 0$ which enables us to integrate out both quark and gauge degrees of freedom \([3]\). The resulting dual representation is then sampled by using the worm algorithm \([4]\). Besides the nuclear potential, we will also calculate the baryon mass $m_{B}$ and study its dependence on finite size effects and temperature. In addition, we will compute the influence of a baryon on the energy density of the surrounding meson cloud and compare it to the nuclear potential and the free boson propagator on the lattice.
2 Lattice Quantum Chromodynamics

2.1 Continuum Lagrangian

Before we start discretizing QCD on the lattice, we will review the continuum formulation by constructing the Lagrangian in Minkowski space. As mentioned in the introduction, quarks are massive spin-$\frac{3}{2}$ fermions. Thus they are described by Dirac-spinors

$$\bar{\psi}^{(f)}(x), \psi^{(f)}(x),$$

where $f = 1, \ldots, N_f = 6$ denotes the flavor and $x$ the 4-position in Minkowski space. $\bar{\psi}$ is the Dirac-adjoint spinor and is related to $\psi$ by $\bar{\psi} = \psi^\dagger \gamma_0$. In addition to spin, quarks carry another internal degree of freedom, the color, which can take three different values: red (r), blue (b) and green (g). To avoid more indices, we will use matrix-vector notation for spin and color degrees of freedom. In absence of an external field, the quark fields fulfill the Dirac equation

$$\left( i \gamma^\mu \partial_\mu - m \right) \psi(x) = 0, \quad (2.1.1)$$

where $m$ is the quark mass and $\gamma_\mu$ are the Dirac matrices. They obey the anti-commutation relation

$$\{ \gamma_\mu, \gamma_\nu \} = 2 \eta_{\mu\nu} \mathbb{1}. \quad (2.1.2)$$

The Lagrangian leading to (2.1.1) can be written as

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi} \left( i \gamma^\mu \partial_\mu - m \right) \psi, \quad (2.1.3)$$

which is easily seen by plugging in (2.1.3) into the Euler-Lagrange equation

$$\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial \left( \partial_\mu \psi \right)} \right) = 0$$

while substituting $\phi$ with $\bar{\psi}$. As there are no expressions in (2.1.3) acting on the color-space, $\mathcal{L}_{\text{Dirac}}$ is invariant under unitary transformations of $\psi$ such as

$$\psi \to \psi' = \Omega \psi$$
$$\bar{\psi} \to \bar{\psi}' = \bar{\psi} \Omega^\dagger, \quad \Omega \in U(3).$$

Having in mind the gauge group of QCD, we restrict to transformations $\Omega \in SU(3)$ and choose $\Omega = \Omega(x)$ to be x-dependent. Demanding invariance under these local gauge transformations then requires the introduction of gauge fields $A^a_\mu$ and a covariant derivative

$$D_\mu = \partial_\mu - ig_\ast T^a A^a_\mu. \quad (2.1.4)$$

Here, $g_\ast$ is the coupling constant of the strong interaction and $T^a$ is the a’th generator of $SU(3)$ with $a = 1, 2, \ldots, 8$. The Generators $T$ fulfill the commutation relation

$$[T^a, T^b] = if^{abc} T^c, \quad (2.1.5)$$
2.1 Continuum Lagrangian

where \( f^{abc} \) is the structure constant of \( SU(3) \). Replacing \( \partial_\mu \) in (2.1.3) by the covariant derivative, the Lagrangian for interacting quarks becomes

\[
\mathcal{L}_q = \bar{\psi} (i\gamma^\mu D_\mu - m) \psi. \tag{2.1.6}
\]

To obtain local gauge invariance for (2.1.6), \( D_\mu \) has to transform covariantly:

\[
D'_\mu \psi^I(x) = \left( \partial_\mu - i g_s T^a A_\mu^a \right) \psi^I(x) = \left( \partial_\mu + \Omega^I(x) \partial_\mu \Omega(x) - i g_s \Omega^I(x) T^a A_\mu^a \Omega(x) \right) \psi^I(x)
\]

\[
= \Omega(x) \left( \partial_\mu + \Omega^I(x) \partial_\mu \Omega(x) - i g_s \Omega^I(x) T^a A_\mu^a \Omega(x) \right) \psi^I(x)
\]

\[
= \frac{1}{\Omega(x)} \Omega(x) D_\mu \psi(x).
\]

This equation is fulfilled if the gluon fields transform inhomogeneously via [5]

\[
T^a A_\mu^a(x) = \Omega(x) \left( T^a A_\mu^a(x) - \frac{1}{g_s} \Omega(x)^\dagger \partial_\mu \Omega(x) \right) \Omega(x)^\dagger.
\]

The kinetic term for the gluons can be constructed in analogy to QED, where the field strength tensor \( F_{\mu\nu} \) is defined as \( F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \) and \( \mathcal{L}_{\text{gauge}} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \). This field strength tensor is related to the covariant derivative of QED by

\[
[D_\mu, D_\nu] = i e F_{\mu\nu}. \tag{2.1.7}
\]

Here, \( e \) is the elementary charge [5]. We can use this commutation relation to find the field strength tensor for QCD by calculating \([D_\mu, D_\nu]\) for the covariant derivative defined in (2.1.4)

\[
[D_\mu, D_\nu] \psi(x) = \left( \left( \partial_\mu - i g_s T^a A_\mu^a \right) \left( \partial_\nu - i g_s T^b A_\nu^b \right) - \left( \partial_\nu - i g_s T^b A_\nu^b \right) \left( \partial_\mu - i g_s T^a A_\mu^a \right) \right) \psi(x)
\]

\[
= -i g_s \left( T^a (\partial_\mu A_\nu^a) - T^a (\partial_\nu A_\mu^a) - i g_s \left[ T^a, T^b \right] A_\mu^a A_\nu^b \right) \psi(x)
\]

\[
= -i g_s \left( T^a (\partial_\mu A_\nu^a) - T^a (\partial_\nu A_\mu^a) + g_s f^{abc} T^a A_\mu^b A_\nu^c \right) \psi(x)
\]

\[
= -i g_s T^a F_{\mu\nu}^a \psi(x).
\]

In the second line, we used the product rule and the fact that \( \partial_\mu \partial_\nu \psi(x) = \partial_\nu \partial_\mu \psi(x) \) such that derivatives of \( \psi(x) \) cancel each other and made use of (2.1.5) in the third line. In the last line, we defined the field strength tensor for QCD by

\[
F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f^{abc} A_\mu^b A_\nu^c. \tag{2.1.8}
\]

With (2.1.8) at hand, we can formulate the kinetic term of the gluons

\[
\mathcal{L}_{\text{gluons}} = -\frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu}. \tag{2.1.9}
\]

Summing up the six different quark flavors, the full Lagrangian of QCD in Minkowski space is now given by

\[
\mathcal{L}_{QCD} = -\frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu} + \sum_{f=1}^{N_f} \bar{\psi}^{(f)} \left( i \gamma^\mu D_\mu - m^{(f)} \right) \psi^{(f)}. \tag{2.1.10}
\]

Apart from the color index \( a \) and the sum over the quark flavors, this Lagrangian has the same form as the QED Lagrangian. However, the dynamics described by (2.1.10) is completely different. The additional term \( g_s f^{abc} A_\mu^b A_\nu^c \) in the field strength tensor leads to new interactions absent in QED. From (2.1.9) 3-gluon and 4-gluon vertices, describing gluon self-interactions, can be read off. These self-interactions are conjectured to be responsible for confinement.
2.2 Path integral formalism

We now want to highlight the basic idea of the path integral formalism. For simplicity, we will first consider non-relativistic quantum mechanics in one spatial dimension and give the corresponding quantities in QFT later.

In non-relativistic quantum mechanics, given the initial state $|\psi_i, t_i\rangle$ at time $t_i$, the final state $|\psi_f, t_f\rangle$ at a later time $t_f$ is usually determined by solving the Schrödinger equation. In the path integral formulation, however, the final state can be calculated directly by using the so-called propagator $K(q_f, t_f; q_i, t_i)$. It is defined such that

$$
\Psi(q_f, t_f) = \int dq_i K(q_f, t_f; q_i, t_i)\Psi(q_i, t_i).
$$

(2.2.1)

From (2.2.1) it is clear that $|K(q_f, t_f; q_i, t_i)|^2$ is the probability for a transition from $(q_i, t_i)$ to $(q_f, t_f)$, concluding that $K(q_f, t_f; q_i, t_i) = \langle q_i, t_i|q_f, t_f\rangle$ (see chapter 5 of [6] for details).

Now we want to express the propagator as a path integral. For that purpose, we split the time interval between $t_f$ and $t_i$ by introducing an intermediate step $(q, t)$. Applying (2.2.1) two times leads to

$$
\Psi(q_f, t_f) = \int dq_i dq K(q_f, t_f; q, t)K(q, t; q_i, t_i)\Psi(q_i, t_i),
$$

which implies

$$
K(q_f, t_f; q_i, t_i) = \int dq K(q_f, t_f; q, t)K(q, t; q_i, t_i).
$$

(2.2.2)

With this identity at hand, we split $[t_i, t_f]$ into $n + 1$ parts of length $\tau$ resulting in

$$
\langle q_f t_f |q_i t_i\rangle = \int \ldots \int dq_1 dq_2 \ldots dq_n \left\langle q_f t_f |q_{n+1}\right\rangle \left\langle q_{n+1} t_{n+1} |q_{n-1} t_{n-1}\right\rangle \ldots \left\langle q_1 t_1 |q_i t_i\right\rangle .
$$

(2.2.3)

By supposing that $\tau \ll 1$ and using $|qt\rangle = \exp(-i\hat{H}t/\hbar)|q\rangle$, the matrix elements $\left\langle q_{i+1} t_{i+1} |q_i t_i\right\rangle$ can be evaluated further, leading to

$$
\left\langle q_{i+1} t_{i+1} |q_i t_i\right\rangle = \left\langle q_i |e^{-i\hat{H}\tau/\hbar}\right|q_i\rangle = \left\langle q_i\left|1 - \frac{i}{\hbar} \hat{H}\tau + \mathcal{O}(\tau^2)\right|q_i\right\rangle
$$

$$
= \delta(q_{i+1} - q_i) - \frac{i\tau}{\hbar} \left\langle q_i |\hat{H}|q_i\right\rangle
$$

$$
= \frac{1}{2\pi\hbar} \int dp \exp\left[\frac{i}{\hbar} p(q_{i+1} - q_i)\right] - \frac{i\tau}{\hbar} \left\langle q_i |\hat{H}|q_i\right\rangle ,
$$

where we used the orthogonality of the position states in the second line and the Fourier transform of the $\delta$-function in the third line [6].

If we assume that $\hat{H}$ is of the form $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$, the remaining matrix element $\left\langle q_{i+1} |\hat{H}|q_i\right\rangle$
2.2 Path integral formalism

can be determined. Using completeness of states $\int |q_i t_i\rangle \langle q_i t_i| \, dq_i = \text{id.}$, we write

\[
\langle q_{i+1} | \frac{\hat{p}^2}{2m} | q_i \rangle = \int dp' dp \langle q_{i+1} | p' \rangle \langle p' | \frac{\hat{p}^2}{2m} | p \rangle \langle p(q_i) = \int \frac{dp' dp}{2\pi \hbar} \exp \left[ \frac{i}{\hbar} (p' q_{i+1} - p q_i) \right] \frac{p^2}{2m} \delta (p - p') = \int \frac{dp}{2\pi \hbar} \exp \left[ \frac{i}{\hbar} p(q_{i+1} - q_i) \right] \frac{p^2}{2m} .
\]

Going from the first to the second line, we used that $\langle p' | \frac{\hat{p}^2}{2m} | p \rangle = \frac{p^2}{2m} \delta (p - p')$ and $\langle q_{i+1} | p' \rangle = (2\pi \hbar)^{-\frac{1}{2}} \exp (i p' q_{i+1} / \hbar)$. Going from the second to the third line, we exploited the $\delta$-function to eliminate the $p'$ integral. The matrix element containing the potential $V(q)$ is given by

\[
\langle q_{i+1} | V(\bar{q}) | q_i \rangle = \langle q_{i+1} \left| V \left( \frac{q_{i+1} + q_i}{2} \right) \right| q_i \rangle = V \left( \frac{q_{i+1} + q_i}{2} \right) \delta (q_{i+1} - q_i) = \int dp \exp \left[ \frac{i}{\hbar} p(q_{i+1} - q_i) \right] V \left( \frac{q_{i+1} + q_i}{2} \right) .
\]

By combining both parts, we arrive at

\[
\langle q_{i+1} | \hat{H} | q_i \rangle = \int \frac{dp}{2\pi \hbar} \exp \left[ \frac{i}{\hbar} p(q_{i+1} - q_i) \right] H(p, q) .
\]

Note that (2.2.4) depends on the classical Hamiltonian $H(p, q)$ and the integral on the right hand side contains no operators. Now the matrix element $\langle q_{i+1} t_{i+1} | q_i t_i \rangle$ simplifies to

\[
\langle q_{i+1} t_{i+1} | q_i t_i \rangle = \frac{1}{2\pi \hbar} \int dp_i \exp \left\{ \frac{i}{\hbar} \left[ p_i (q_{i+1} - q_i) - \tau H(p_i, \bar{q}_i) \right] \right\} , \quad \text{with} \quad \bar{q}_i = \frac{q_{i+1} + q_i}{2} .
\]

Following the arguments in chapter 5 of [6], we obtain the complete propagator by inserting this result into (2.2.3), performing the momentum integration and taking the limit $n \to \infty$:

\[
\langle q_f t_f | q_i t_i \rangle = \lim_{n \to \infty} \int \left[ \prod_{i=1}^{n} dq_i \right] \left[ \prod_{i=0}^{n} dp_i \right] \exp \left\{ \frac{i}{\hbar} \sum_{i=0}^{n} \left[ p_i (q_{i+1} - q_i) - \tau H(p_i, \bar{q}_i) \right] \right\} = \lim_{n \to \infty} \int \left[ \prod_{i=1}^{n} dq_i \right] \left[ \prod_{i=0}^{n} dp_i \right] \exp \left\{ \frac{i}{\hbar} \sum_{i=0}^{n} \left[ p_i (q_{i+1} - q_i) - \frac{p_i^2}{2m} - \tau V(q_i) \right] \right\} = \lim_{n \to \infty} \left( \frac{m}{\hbar \tau} \right)^{n+\frac{1}{2}} \int \left[ \prod_{i=1}^{n} dq_i \right] \exp \left\{ \frac{i \tau}{\hbar} \sum_{i=0}^{n} \left[ \frac{m}{2} \left( \frac{q_{i+1} - q_i}{\tau} \right)^2 - V(q_i) \right] \right\} = N \int_{q_i}^{q_f} \mathcal{D}q \exp \left[ \frac{i}{\hbar} \int_{t_i}^{t_f} L(q, \dot{q}) dt \right] = N \int_{q_i}^{q_f} \mathcal{D}q \exp \left[ \frac{i}{\hbar} S[q, \dot{q}] \right] .
\]
The integration in the third line was performed by using (A.3.1). Note that $\frac{q_{i+1} - q_i}{\tau} = \dot{q}(t) + O(\tau)$ with $t = i\tau$. In the same way, the sum over $n$ is an approximation of an integral from $t_i$ to $t_f$. By taking the limit $n \to \infty$, we arrive at line four where $L(q, \dot{q}) = \frac{m}{2} \dot{q}^2 - V(q)$ is the classical Lagrangian of the system. The measure $Dq$ and the normalization constant $N$ are symbolical notations for $\prod_{i=1}^n dq_i$ and $(\frac{m}{i\hbar})^{n+\frac{1}{2}}$ in the limit $n \to \infty$. In the last line, the definition of the action as the integral over the Lagrangian was used.

We can now switch to imaginary time $t = i\tau$, $\tau \in \mathbb{R}$ and express the path integral by the Euclidean action as

$$
\langle q_{tf}|q_{ti}\rangle = N \int_{q_i}^{q_f} Dq \exp \left[ i \frac{1}{\hbar} \int_{t_i}^{t_f} L(q(\tau), \dot{q}(\tau)) d\tau \right] = N \int_{q_i}^{q_f} Dq \exp \left[ \frac{i}{\hbar} \int_{t_i}^{t_f} L_E(q(t), \dot{q}(t)) dt \right] = N \int_{q_i}^{q_f} Dq \exp \left[ -\frac{1}{\hbar} S_E[q, \dot{q}] \right].
\tag{2.2.6}
$$

In contrast to the oscillatory behavior of the path integral in real time, (2.2.6) is now exponentially damped. By changing the boundary conditions to periodic ones, i.e. $q_f \equiv q_i$, we can also express the partition function as a path integral (see chapter 1 of [7]).

$$
Z_T = \text{tr} \left[ e^{-T\hat{H}} \right] = \int dq \langle q| e^{-T\hat{H}} |q\rangle = N \int Dq \exp \left[ -\frac{1}{\hbar} S_E[q, \dot{q}] \right],
\tag{2.2.7}
$$

The concept of a path integral is also used in quantum field theory and in analogy to (2.2.7), the partition function can be written as

$$
Z = \int D\phi \ e^{-S_E[\phi]}.
\tag{2.2.8}
$$

The expectation value of an operator $\hat{O}$ is then given by

$$
\langle \hat{O} \rangle = \frac{1}{Z} \int D\phi \ O[\phi] \ e^{-S_E[\phi]}.
\tag{2.2.9}
$$

Similar to the non-relativistic quantum mechanic case, $S_E[\phi]$ and $O[\phi]$ are functionals of the classical fields $\phi$. There are no operator-valued expressions on the right hand side of (2.2.8) and (2.2.9).

### 2.3 Lattice discretization

We aim to evaluate expectation values like (2.2.9) using numerical simulations. As it is impossible to perform this infinite dimensional integration directly with a computer, we have to find a suitable approximation for (2.2.9). When deriving the propagator for the one dimensional quantum mechanic case, we already encountered such an approximation. We separated the time axis into $n+1$ segments of length $\tau$ and performed an expansion valid for small $\tau$. At the
2.3 Lattice discretization

end of the calculation, we took the continuum limit \( n \to \infty \) such that this expansion became exact. So instead of taking \( n \to \infty \), we can use the expression at finite \( n \) to define a path integral of resolution \( \tau \) that can be evaluated numerically.

For 3+1 dimensional QCD, this suggests to discretize spacetime onto a four dimensional lattice with a lattice spacing \( a \) and to find a lattice version of the action which approaches the continuum formulation in the limit \( a \to 0, |\Lambda| \to \infty \), where \( |\Lambda| \) is the number of lattice sites.

We do so by defining

\[
\Lambda := \{ n = (n_1, n_2, n_3, n_4) | n_1, n_2, n_3 = 0, 1, \ldots, N_\sigma - 1; n_4 = 0, 1, \ldots, N_\tau - 1 \},
\]

(2.3.1)

where \( N_\sigma \) is the spatial and \( N_\tau \) the temporal lattice extent. The physical position corresponding to \( n \) is then \( x = an \). The quark fields \( \psi, \bar{\psi} \) are now defined on the lattice sites

\[
\psi(n), \bar{\psi}(n); \ n \in \Lambda.
\]

The next step is to formulate the lattice version of the Euclidean QCD action. We start by discretizing the action for free quarks. In the continuum, it is given by

\[
S_E[\bar{\psi}, \psi] = \int d^4 x \ L_E(\bar{\psi}, \psi) = \int d^4 x \bar{\psi}(x) (\gamma_\mu \partial_\mu + m) \psi(x).
\]

(2.3.2)

Note that the Euclidean Lagrangian differs from the Minkowski formulation in (2.1.3). Here, the mass carries a positive sign and the factor \( i \) in front of the derivative dropped. In addition, the \( \gamma_\mu \)-matrices occurring here are not the same as in (2.1.3). They fulfill a different anti-commutation relation, namely

\[
\{\gamma_\mu, \gamma_\nu\} = 2 \delta_{\mu\nu} \mathbb{1}.
\]

Replacing the partial derivatives in (2.3.2) by central differences

\[
\partial_\mu \psi(x) \to \frac{1}{2a} (\psi(n + \hat{\mu}) - \psi(n - \hat{\mu}))
\]

and the integral by a sum over all lattice sites

\[
\int d^4 x \to a^4 \sum_{n \in \Lambda},
\]

we arrive at

\[
S_{\text{free}} = a^4 \sum_{n \in \Lambda} \bar{\psi}(n) \left( \sum_{\mu=1}^4 \frac{\gamma_\mu}{2a} [\psi(n + \hat{\mu}) - \psi(n - \hat{\mu})] + m\psi(n) \right).
\]

(2.3.3)

In analogy to section 2.1, we can construct the interacting fermion action by requiring invariance under local \( SU(3) \) transformations. Applying the transformations

\[
\psi(n) \to \Omega(n) \psi(n), \ \Omega(n) \in SU(3)
\]

(2.3.4)

\[
\bar{\psi}(n) \to \bar{\psi}(n) \Omega(n)^\dagger
\]

(2.3.5)
2 Lattice Quantum Chromodynamics

to $S_{\text{free}}$ leads to

$$S_{\text{free}} \rightarrow S'_{\text{free}} = a^4 \sum_{n \in \Lambda} \bar{\psi}(n) \Omega(n) \epsilon$$

$$\times \left( \sum_{\mu=1}^{4} \frac{\gamma_{\mu}}{2a} \left[ \Omega(n + \hat{\mu}) \psi(n + \hat{\mu}) - \Omega(n - \hat{\mu}) \psi(n - \hat{\mu}) \right] + m \Omega(n) \psi(n) \right).$$

Apparently, the derivative term is not gauge invariant. To overcome this, we introduce group valued gauge fields $U_{\mu}(n)$, which transform according to

$$U_{\mu}(n) \rightarrow U'_{\mu}(n) = \Omega(n) U_{\mu}(n) \Omega(n + \hat{\mu})^{\dagger}, \quad U_{\mu} \in SU(3). \quad (2.3.6)$$

We also define

$$U_{-\mu}(n) \equiv U_{\mu}(n - \hat{\mu})^{\dagger}, \quad (2.3.7)$$

such that

$$U_{-\mu}(n)' = (U_{\mu}(n - \hat{\mu})')^{\dagger} = \left( \Omega(n - \hat{\mu}) U_{\mu}(n - \hat{\mu}) \Omega(n) \right)^{\dagger}$$

$$= \Omega(n) U_{\mu}(n - \hat{\mu})^{\dagger} \Omega(n - \hat{\mu})^{\dagger} = \Omega(n) U_{-\mu}(n) \Omega(n - \hat{\mu})^{\dagger}. \quad (2.3.10)$$

These gauge fields are oriented and connect two neighboring lattice sites. They are therefore often called link variables. With the link variables at hand, we can formulate the so-called naive fermion action

$$S_{\text{naive}} = a^4 \sum_{n \in \Lambda} \bar{\psi}(n) \left( \sum_{\mu=1}^{4} \frac{\gamma_{\mu}}{2a} \left[ U_{\mu}(n) \psi(n + \hat{\mu}) - U_{-\mu}(n) \psi(n - \hat{\mu}) \right] + m \psi(n) \right). \quad (2.3.8)$$

The invariance of $S_{\text{naive}}$ under gauge transformations then follows directly from (2.3.6) and (2.3.7).

From these transformation properties, one can relate the lattice gauge fields $U_{\mu}(n) \in SU(3)$ to the continuum fields $A_{\mu}(x) \in su(3)$. In the continuum, the same transformation properties are fulfilled by the so-called path-ordered gauge transporter $[8]$

$$G(x, y) = P \exp \left( \frac{i}{\hbar} \int_{C} A \cdot ds \right), \quad (2.3.9)$$

which transforms according to

$$G(x, y) \rightarrow G(x, y)' = \Omega(x) G(x, y) \Omega(y)^{\dagger}. \quad (2.3.10)$$

By introducing algebra valued lattice gauge fields $A_{\mu}(n)$ via

$$U_{\mu}(n) = \exp \left( ia A_{\mu}(n) \right) \quad (2.3.11)$$

and comparing it to (2.3.9), we see that $U_{\mu}(n)$ is an approximation of $G(n, n + \hat{\mu})$ to $O(a)$. 

8
A simple lattice version of the Yang-Mills action is given by the so-called Wilson gauge action \[ S_G[U] = \frac{\beta}{N_c} \sum_{n \in \Lambda} \sum_{\nu < \mu} \text{Re} \text{tr} [1 - U_{\mu\nu}(n)], \] (2.3.12)

where \( \beta = \frac{2N_c}{g_s^2} \) and \( U_{\mu\nu}(n) \) is the elementary plaquette defined by

\[ U_{\mu\nu}(n) = U_\mu(n)U_\nu(n + \hat{\mu})U_{-\mu}(n + \hat{\mu} + \hat{\nu})U_{-\nu}(n + \hat{\nu}). \] (2.3.13)

A sketch of such an elementary plaquette is given in Fig. 1.

![Figure 1: The elementary plaquette U_{\mu\nu}(n) as defined in (2.3.12). The orientations of the link variables are indicated by arrows.](image)

2.4 Doubling problem

Starting from the naive fermion action (2.3.8), we want to calculate the quark propagator and investigate its poles in momentum space to see which particles are described by the action. \( S_{\text{naive}} \) can be rewritten by defining the naive Dirac operator \( D(n|m)^{\alpha\beta}_{ab} \) such that

\[ S_{\text{naive}} = a^4 \sum_{n,m \in \Lambda} \sum_{a,b,\alpha,\beta} \bar{\psi}(n)^{\alpha}_{a} D(n|m)^{\alpha\beta}_{ab} \psi(m)^{\beta}_{b}, \]

where

\[ D(n|m)^{\alpha\beta}_{ab} = \sum_{\mu=1}^{4} \left( \frac{\gamma_\mu}{2a} \right)^{\alpha\beta} \left( U_\mu(n)_{ab} \delta_{n+\hat{\mu},m} - U_{-\mu}(n)_{ab} \delta_{n-\hat{\mu},m} \right) + m \delta^{\alpha\beta} \delta_{ab} \delta_{n,m}. \] (2.4.1)
2 Lattice Quantum Chromodynamics

Considering the free case $U_\mu = 1$ and dropping the Dirac and color indices for notational convenience, the discrete Fourier transform of $D(n|m)$ is

$$
\tilde{D}(p|q) = \frac{1}{|A|} \sum_{n,m \in A} e^{-ip \cdot na} D(n|m)e^{iq \cdot ma}
$$

$$
= \frac{1}{|A|} \sum_{n,m \in A} e^{-ip \cdot na} \left( \sum_{\mu=1}^{4} \gamma_\mu \frac{\delta_{n+\hat{\mu},m} - \delta_{n-\hat{\mu},m}}{2a} + i m \delta_{n,m} \right) e^{iq \cdot ma}
$$

$$
= \frac{1}{|A|} \sum_{n \in A} e^{-ip \cdot na} \left( \sum_{\mu=1}^{4} \gamma_\mu \frac{e^{i\pi(\mu+\hat{\mu})a} - e^{i\pi(\mu-\hat{\mu})a}}{2a} + i m \right)
$$

$$
= \frac{1}{|A|} \sum_{n \in A} e^{-i(p-q) \cdot na} \left( \sum_{\mu=1}^{4} \gamma_\mu \frac{e^{i\pi \mu a} - e^{-i\pi \mu a}}{2a} + i m \right)
$$

$$
\equiv \delta(p-q) \tilde{D}(q),
$$

where $\tilde{D}(q) = \frac{1}{a} \sum_{\mu=1}^{4} \gamma_\mu \sin(q_\mu a)$ was defined in the last line. Since $\gamma_\mu = \gamma_\mu^{-1}$, multiplying $\tilde{D}(p)$ with $\frac{1}{a} \sum_{\mu=1}^{4} \gamma_\mu \sin(p_\mu a)$ leads to

$$
\left( \frac{1}{a} \sum_{\mu=1}^{4} \gamma_\mu \sin(p_\mu a) \right) \cdot \left( \frac{1}{a} \sum_{\mu=1}^{4} \gamma_\mu \sin(p_\mu a) \right) = m^2 + \frac{1}{a^2} \sum_{\mu=1}^{4} \sin(p_\mu a)^2.
$$

From here, the inverse $\tilde{D}(p)^{-1}$ is given by

$$
\tilde{D}(p)^{-1} = \frac{\frac{1}{a} \sum_{\mu=1}^{4} \gamma_\mu \sin(p_\mu a)}{m^2 + \frac{1}{a^2} \sum_{\mu=1}^{4} \sin(p_\mu a)^2}.
$$

The quark propagator can now be expressed via $\tilde{D}(p)^{-1}$ by inverting the Fourier transformation and exploiting the $\delta$-function in (2.4.2). It then reads

$$
D^{-1}(n|m) = \frac{1}{|A|} \sum_{p \in A} \tilde{D}(p)^{-1} e^{ip \cdot (n-m)a}.
$$

By setting $m = 0$ for simplicity, the poles of (2.4.3) can be read off. They are located at

$$
P = (0, 0, 0, 0), \left( \frac{\pi}{a}, 0, 0, 0 \right), \left( 0, \frac{\pi}{a}, 0, 0 \right), \ldots, \left( \frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a} \right).
$$

Counting all combinations together, we arrive at 16 poles, corresponding to 16 particle states instead of just one. Of these, only the pole at $P = (0, 0, 0, 0)$ is the physical pole for a massless fermion. It is also present in the continuum Dirac operator. The other 15 poles, each containing $\frac{\pi}{a}$ in some components, are unphysical. These are called doubleers. We therefore see that the naive approach suffers from large lattice artifacts and is not suitable for our simulations.
2.5 Staggered fermions

As the discretization of the action is not unique, many different actions have been proposed, all stemming from the aim of minimizing lattice artifacts. One such discretization is the staggered fermion action, which reduces the number of degenerate particle states from 16 to four while leaving chiral symmetry intact. The basic idea is to transform the quark fields such that the \( \gamma_\mu \)-matrix in the first term of the naive fermion action \( (2.3.8) \) is canceled. The action resulting from this staggered transformation is then diagonal in Dirac-space and three of the four Dirac-indices are omitted.

The transformed quark fields \( \phi, \bar{\phi} \) are defined by

\[
\psi(n) = \gamma_1^n \gamma_2^{n_2} \gamma_3^{n_3} \gamma_4^{n_4} \phi(n), \quad \bar{\psi}(n) = \bar{\phi}(n) \gamma_4^{n_4} \gamma_3^{n_3} \gamma_2^{n_2} \gamma_1^n .
\]  

(2.5.1)

Applying this transformation to the mass term of \( (2.3.8) \) leads to even powers of \( \gamma_\mu \)-matrices and since \( \gamma_\mu^2 = 1 \), it follows that

\[
m\bar{\psi}(n)\psi(n) = m\bar{\phi}(n)\gamma_4^{n_4} \gamma_3^{n_3} \gamma_2^{n_2} \gamma_1^n \phi(n) = m\bar{\phi}(n)\phi(n).
\]

In the kinetic term, we encounter products where the \( \psi \)-field is shifted by a lattice constant such that

\[
\bar{\psi}(n)\gamma_\mu \psi(n \pm \mu) = \bar{\phi}(n)\gamma_4^{n_4} \gamma_3^{n_3} \gamma_2^{n_2} \gamma_1^n \gamma_\mu^{n_1+\delta_{\mu_1}} \gamma_2^{n_2+\delta_{\mu_2}} \gamma_3^{n_3+\delta_{\mu_3}} \gamma_4^{n_4+\delta_{\mu_4}} \phi(n \pm \mu) = \eta_\mu(n)\bar{\phi}(n)\bar{\phi}(n \pm \mu).
\]

In the last line, the staggered sign functions

\[
\eta_\mu(n) = (-1)^{\sum_{\nu < \mu} n_\nu}
\]  

(2.5.2)

were defined. They represent the staggered version of the \( \gamma \)-matrices. By defining new fields \( \tilde{\chi}, \tilde{\bar{\chi}} \) as single Dirac-components of \( \bar{\phi}, \phi \) and introducing the gauge fields \( U_\mu \), the staggered fermion action reads

\[
S_{\text{stag}} = a^4 \sum_{n \in \Lambda} \tilde{\chi}(n) \left( \sum_{\mu=1}^{4} \frac{\eta_\mu(n)}{2a} \left[ U_\mu(n)\tilde{\chi}(n + \mu) - U_{-\mu}(n)\tilde{\chi}(n - \mu) \right] + m\tilde{\chi}(n)\tilde{\chi}(n) \right).
\]  

(2.5.3)

Furthermore, we can define dimensionless fields \( \chi(n) = i\sqrt{2}a^{3/2}\tilde{\chi}(n) \) to obtain

\[
S_{\text{stag}} = -\sum_{n \in \Lambda} \left( \sum_{\mu=1}^{4} \eta_\mu(n) \left[ \tilde{\chi}(n)U_\mu(n)\chi(n + \mu) - \tilde{\chi}(n + \mu)U_\mu(n)^\dagger\chi(n) \right] + 2am\tilde{\chi}(n)\chi(n) \right).
\]  

(2.5.4)

\[1\]Dirac and lattice indices are mixed by the staggered transformation. To obtain the usual spinor structure, the lattice is separated into hypercubes and the fields contained in such a hypercube are grouped together, forming new quark fields (see chapter 10 of [3] for further details).
2.6 Temperature, anisotropic coupling and chemical potential

So far, our considerations were restricted to both zero temperature and chemical potential. To include a non-zero temperature into a continuum field theory, we have to change the region of integration of the action from

$$S_E = \int_{\mathbb{R}^4} d^4x \mathcal{L}_E(\bar{\psi}, \psi)$$

to

$$S_E(T) = \int_0^\beta dt \int_{\mathbb{R}^3} d^3x \mathcal{L}_E(\bar{\psi}, \psi),$$

where $\beta = \frac{1}{T}$. The integration is now restricted to a finite temporal extent. On the lattice, we would have to change the definition of our action accordingly but we already took care of this issue in (2.3.1) as we separated spatial and temporal lattice sizes. The temperature is related to the temporal lattice spacing via

$$\beta = aN_T = \frac{1}{T}. \quad (2.6.2)$$

Keeping a fixed temperature on the lattice also influences the way we have to take the continuum limit. Instead of taking $a \to 0$, $|\Lambda| \to \infty$, we now have to take $a \to 0$ while keeping $a|\Lambda|$ and $aN_T$ fixed. According to (2.6.2), $T$ can only be varied in discrete steps if the lattice spacing $a$ is fixed. This restriction can be avoided by introducing an anisotropic coupling $\gamma$ such that

$$S_{stag} = -\sum_{n \in \Lambda} \left( \sum_{\mu=1}^3 \eta_\mu(n) \left[ \bar{\chi}(n)U_\mu(n)\chi(n + \hat{\mu}) - \bar{\chi}(n + \hat{\mu})U_\mu^\dagger(n)\chi(n) \right] 
+ \eta_4(n)\gamma \left[ \bar{\chi}(n)U_4(n)\chi(n + \hat{4}) - \bar{\chi}(n + \hat{4})U_4^\dagger(n)\chi(n) \right] + 2am\bar{\chi}(n)\chi(n) \right).$$

Temporal and spatial hoppings couple differently at $\gamma \neq 1$ so a distinction between temporal and spatial lattice spacings is introduced. This enables us to define the physical anisotropy $\xi(\gamma) = \frac{a}{aN_T}(\gamma)$. The temperature can now be written as

$$aT = \frac{\xi(\gamma)}{N_T}, \quad (2.6.3)$$

and can be varied continuously by changing $\gamma$. Furthermore, we can include a quark chemical potential $\mu_q$ in the fermion action. This changes the temporal gauge links by

$$U_4(n) \to e^{a_\tau \mu_q} U_4(n), \quad (2.6.4)$$
$$U_4(n)\dagger \to e^{-a_\tau \mu_q} U_4^\dagger(n). \quad (2.6.5)$$

This is important in the strong coupling limit $\beta_{\text{coupling}} = \frac{2N_c}{g_s^2} = 0$ since $\beta_{\text{coupling}}$ cannot be used to vary $T$.\footnote{This is important in the strong coupling limit $\beta_{\text{coupling}} = \frac{2N_c}{g_s^2} = 0$ since $\beta_{\text{coupling}}$ cannot be used to vary $T$.}
With these modified links, the staggered fermion action at $\gamma \neq 1$ becomes

$$S_{stag} = -\sum_{n \in \Lambda} \left( \sum_{\mu=1}^{3} \eta_{\mu}(n) \left[ \bar{\chi}(n) U_\mu(n) \chi(n + \hat{\mu}) - \bar{\chi}(n + \hat{\mu}) U_\mu^\dagger(n) \chi(n) \right] ight)$$

$$+ \eta_{4}(n) \gamma \left[ \bar{\chi}(n) e^{a_{\tau} U_4(n)} \chi(n + \hat{4}) - \bar{\chi}(n + \hat{4}) e^{-a_{\tau} U_4^\dagger(n)} \chi(n) \right] + 2am \bar{\chi}(n) \chi(n).$$  
{(2.6.6)}

This formulation of lattice fermions will be used throughout the rest of this thesis. With it, we can now formulate the partition function for lattice QCD in terms of a (lattice-)path integral

$$Z_{lat} = \int D[\bar{\chi}] D[\chi] D[U] e^{-S_{stag}[\bar{\chi},\chi,U] - S_{G}[U]}, \quad \text{with}$$

$$D[\bar{\chi}] = \prod_{n \in \Lambda} d\bar{\chi}(n), \quad D[\chi] = \prod_{n \in \Lambda} d\chi(n), \quad D[U] = \prod_{n \in \Lambda} \prod_{\mu = 1}^{4} dU_\mu(n),$$

where $\bar{\chi}, \chi$ are Grassmann-valued fields and $dU_\mu(n)$ is the Haar measure for $SU(3)$. A short summary of Grassmann numbers and integrals as well as the Haar measure is given in the appendix in A.2 and A.1. The system, described by (2.6.7), is defined on the four dimensional hypercubic lattice $\Lambda$ given in (2.3.1). The boundary conditions in spatial direction are periodic, e.g. $\chi(x, N_\sigma, z, t) = \chi(x, 0, z, t)$. In temporal direction, anti-periodic boundary conditions are imposed: $\chi(x, y, z, N_\tau) = -\chi(x, y, z, 0)$. 
3 The dual representation of SC-LQCD

3.1 Strong coupling limit

As described in [10], a non-zero chemical potential or equivalently a non-zero baryon number leads to the sign problem. The Boltzmann factor becomes complex and hence cannot be used as a probability distribution for importance sampling. Thus, to study the nuclear potential with Monte Carlo methods, we have to tame the sign problem. To do so, we will use an approach that is based on the work of P. Rossi and U. Wolff [11] as well as F. Karsch and K.-H. Mütter [3]. By taking the strong coupling limit $\beta \rightarrow 0$, they were able to perform both the Grassmann and group integration in (2.6.7), resulting in a representation of QCD in terms of discrete degrees of freedom. The sign problem of this new representation is rather mild and can be solved by re-weighting. Although the lattice is infinitely coarse in the strong coupling limit, important properties such as chiral symmetry breaking and confinement are still present.

3.2 One-link integral for $N_f = 1$

By letting $\beta \rightarrow 0$ in (2.6.7), the gauge action (2.3.12) vanishes such that

$$Z = \int \mathcal{D}[\chi] \mathcal{D}[\bar{\chi}] \mathcal{D}[U] e^{-S_F[\chi, \bar{\chi}, U]}.$$ 

Now the integration factorizes and we can write

$$Z = \prod_{n \in \Lambda} \left\{ \int d\chi(n) d\bar{\chi}(n) e^{2am(\bar{\chi}(n)\chi(n))} \prod_{\mu=1}^{4} \left( \int dU_{\mu}(n) e^{\eta_{\mu}(n)(\bar{\chi}(n)U_{\mu}(n)\chi(n+\hat{\mu})-\bar{\chi}(n+\hat{\mu})U_{\mu}^*(n)\chi(n))} \right) \right\}$$

$$= \prod_{n \in \Lambda} \left( \int d\chi(n) d\bar{\chi}(n) e^{2am(\bar{\chi}(n)\chi(n))} \prod_{\mu=1}^{4} z(n, n + \hat{\mu}) \right). \quad (3.2.1)$$

The second line defines the one-link integral which we will calculate for $N_f = 1$ and gauge groups $U(N)$ and $SU(N)$. For simplicity, we will omit the staggered phases $\eta_{\mu}(n)$, the anisotropic coupling $\gamma$ and the chemical potential $\mu_q$ for now and include them later. At first, we note that $z(x, y)$ is of the form

$$z(x, y) = \int_G dg e^{\text{tr}[gm^\dagger + mp]} \quad (3.2.2)$$

if we denote elements of the gauge group by $g \in G$ and define $m$ and $m^\dagger$ to be

$$(m)_{ij} = \chi(x)_i \bar{\chi}(y)_j \quad (3.2.3)$$

$$(m^\dagger)_{ij} = -\chi(y)_i \bar{\chi}(x)_j. \quad (3.2.4)$$

By investigating the behavior of $z(x, y)$ under gauge transformations (Equations (2.3.4), (2.3.5) and (2.3.6), we find

$$z(x, y)' = \int_G dg' e^{\text{tr}[g'm^\dagger + m^\dagger g']} = \int dU_{\mu}' e^{-S_{\text{stag, kin}}[\chi', \bar{\chi}', U'] = \int dU_{\mu} e^{-S_{\text{stag, kin}}[\chi, \bar{\chi}, U]} = z(x, y),$$
where we used the invariance of the kinetic part of \((2.5.4)\) and the property of the Haar measure
\[ dU = d(VU) = d(UV), \quad V \in G. \]

With the invariance of \(z(x, y)\) at hand, we follow the line of arguments given in the appendix of [9] and expand the integral in a series of gauge invariant objects
\[
\begin{align*}
  z(x, y)_{U(N)} &= \sum_{k_1, k_2, \ldots, k_N} \alpha_{k_1, \ldots, k_N} \det[mm]^k_1 \text{tr}[mm]^k_2 \cdots \text{tr}[(mm)^N]^k_N \quad (3.2.5) \\
  z(x, y)_{SU(N)} &= \sum_{k_1, k_2, \ldots, k_{N+1}} \alpha_{k_1, \ldots, k_{N+1}} \det[m]^k_1 \det[m]^k_2 \text{tr}[mm]^{k_3} \cdots \text{tr}[(mm)^N]^k_{N+1}. \quad (3.2.6)
\end{align*}
\]

Note that \(\text{tr}[(mm)^k]\) with \(k \geq N\) can be expressed in terms of determinants and traces of \((mm)^j\) with \(j < N\) by using the Cayley-Hamilton theorem [9]. By defining mesonic variables
\[
M(x) = \sum_{i=1}^{N} \bar{\chi}(x)_i \chi(x)_i \quad (3.2.7)
\]
and computing the product \(M(x)M(y)\), we find
\[
M(x)M(y) = \sum_{i,j=1}^{N} \bar{\chi}(x)_i \chi(x)_i \bar{\chi}(y)_j \chi(y)_j = -\sum_{i,j=1}^{N} \chi(x)_i \bar{\chi}(y)_j \chi(y)_j \bar{\chi}(x)_i = \text{tr}[mm]^i.
\]

Here we used that Grassmann variables anti-commute. In a similar way, it holds that
\[
\text{tr}[(mm)^i] = (-1)^{i+1}(M(x)M(y))^i. \quad (3.2.8)
\]

Using (3.2.8), the expansions of \(z(x, y)\) can be simplified to
\[
\begin{align*}
  z(x, y)_{U(N)} &= \sum_{k} \alpha_k (M(x)M(y))^k, \quad (3.2.9) \\
  z(x, y)_{SU(N)} &= \sum_{i,j,k} \alpha_{ijk} \det[m]^i \det[m]^j \ (M(x)M(y))^k. \quad (3.2.10)
\end{align*}
\]

In the case of \(U(N)\), we made use of the Cayley-Hamilton theorem to express \(\det[mm]^i\) by color traces before applying (3.2.8). For \(SU(N)\) we can define baryonic variables \(B(x), \bar{B}(x)\) by
\[
\begin{align*}
  \det[m] &= \epsilon_{i_1, \ldots, i_n} m_{i_1i_1} \cdots m_{i_Ni_N} = \frac{1}{N!} \epsilon_{i_1, \ldots, i_N} \epsilon_{j_1, \ldots, j_N} m_{j_1i_1} \cdots m_{j_Ni_N} \\
  &\equiv (-1)^N N! \bar{B}(y) B(x). \quad (3.2.11)
\end{align*}
\]
In terms of the staggered quark fields, this translates to

\[ B(x) = \frac{1}{N!} \epsilon_{i_1 \ldots i_N} \chi(x)_{i_1} \cdots \chi(x)_{i_N} \quad (3.2.12) \]

\[ \bar{B}(x) = \frac{1}{N!} \epsilon_{i_1 \ldots i_N} \bar{\chi}(x)_{i_N} \cdots \bar{\chi}(x)_{i_1}. \]

Applying this definition to \( \det[m^1] \) yields

\[ \det[m^1] = N! \bar{B}(x)B(y). \]

Because of the Grassmann property of the \( \chi \)-fields, we see that these determinants can only occur in terms to power one. The product term of those can again be expressed by traces through the Cayley-Hamilton theorem. Similarly, the product \( M(x)M(y) \) can only occur in powers less or equal to \( N \). Thus we can write \( z(x, y) \) as \([9]\)

\[ z(x, y) = \sum_{k=0}^{N} \alpha_k \left( M(x)M(y) \right)^k + \kappa \left( \tilde{\alpha}(-1)^N N! \bar{B}(y)B(x) + \tilde{\beta} N! \bar{B}(x)B(y) \right), \]

\[ \kappa = \begin{cases} 1 & \text{for } SU(N) \\ 0 & \text{for } U(N) \end{cases}. \]

The remaining task is to determine the coefficients \( \alpha_k, \tilde{\alpha} \) and \( \tilde{\beta} \). To obtain \( \tilde{\alpha} \) and \( \tilde{\beta} \), we first expand the exponential function in (3.2.2) in a power series

\[ z(x, y) = \int_G dg \, e^{tr[g m^1 + m^1]} = \sum_{k,l} \frac{1}{k!l!} \int_{SU(N)} dU \left( \bar{\chi}(x)U \chi(y) \right)^k \left( -\bar{\chi}(y)U^\dagger \chi(x) \right)^l, \]

\[ (3.2.14) \]

and compare it to (3.2.13). Using the multinomial theorem \([A.3.2]\) together with the quark fields’ Grassmann property, we see that the \( \bar{B}B \) terms in (3.2.13) are generated by the integrals \( \frac{1}{N!} \int_{SU(N)} dU \left( \bar{\chi}(x)U \chi(y) \right)^N \) and \( \frac{1}{N!} \int_{SU(N)} dU \left( -\bar{\chi}(y)U^\dagger \chi(x) \right)^N \). Therefore we write

\[ \tilde{\beta} N! \bar{B}(x)B(y) = \frac{1}{N!} \int_{SU(N)} dU \left( \bar{\chi}(x)U \chi(y) \right)^N \]

\[ = \frac{1}{N!} \sum_{i_1 \ldots i_N} \sum_{j_1 \ldots j_N} \bar{\chi}(x)_{i_1} \chi(y)_{j_1} \cdots \bar{\chi}(x)_{i_N} \chi(y)_{j_N} \int_{SU(N)} dU \, U_{i_1j_1} \cdots U_{i_Nj_N} \]

\[ = \frac{1}{N! N!} \sum_{i_1 \ldots i_N} \sum_{j_1 \ldots j_N} \epsilon_{i_1 \ldots i_N} \epsilon_{j_1 \ldots j_N} \bar{\chi}(x)_{i_1} \chi(y)_{j_1} \cdots \bar{\chi}(x)_{i_N} \chi(y)_{j_N} \]

\[ = \bar{B}(x)B(y). \]

This implies that \( \tilde{\beta} = \frac{1}{N!} \). The same consideration for \( \bar{B}(y)B(x) \) leads to \( \tilde{\alpha} = \frac{1}{N!} \) \([9]\). The \( SU(N) \) integral that was used in the second line is given in \([A.1.5]\). Now we are left with
computing the coefficients \( \alpha_k \). By plugging in the expanded form (3.2.13) into the identity (A.3.3)

\[
\int d\chi(x) d\bar{\chi}(x) \int dU \, e^{\tilde{\chi}(x)\chi(x) + \tilde{\chi}(x)U\chi(y) - \bar{\chi}(y)U\chi(x)} = e^{\tilde{\chi}(y)\chi(y)},
\]

we obtain

\[
\int d\chi(x) d\bar{\chi}(x) e^{\tilde{\chi}(x)\chi(x)} \sum_{k=0}^{N} \alpha_k (M(x)M(y))^k
\]

\[
= \int d\chi(x) d\bar{\chi}(x) \sum_{l=0}^{N} \frac{1}{l!} (\tilde{\chi}(x)\chi(x))^l \sum_{k=0}^{N} \alpha_k (M(x)M(y))^k
\]

\[
= \int d\chi(x) d\bar{\chi}(x) \sum_{k=0}^{N} \alpha_k \sum_{l=0}^{N-k} \frac{1}{l!} (\tilde{\chi}(x)\chi(x))^{k+l}(\bar{\chi}(y)\chi(y))^k
\]

\[
= \sum_{k=0}^{N} \frac{\alpha_k N!}{(N-k)!} (\bar{\chi}(y)\chi(y))^k.
\]

In the second line, we expanded the exponential function. Then we used the definition (3.2.7) and restricted the \( l \)-sum to \( N - k \) since \( (\tilde{\chi}(x)\chi(x))^l = 0, \quad \forall i > N \). In the last line, we performed the Grassmann integration by using (A.2.7). The factor \( N! \) in the numerator appears due to the multinomial theorem (A.3.2) as \( \tilde{\chi}(x)\chi(x) = \sum_i \tilde{\chi}_i(x)\chi_i(x) \). Equating the last line with the expansion of \( e^{\tilde{\chi}(y)\chi(y)} \), we find

\[
\sum_{k=0}^{N} \frac{\alpha_k N!}{(N-k)!} (\bar{\chi}(y)\chi(y))^k = \sum_{k=0}^{N} \frac{1}{k!} (\bar{\chi}(y)\chi(y))^k
\]

\[
\Rightarrow \alpha_k = \frac{(N-k)!}{N!k!}.
\]

(3.2.15)

Putting all coefficients together, we can write the one-link integral for \( N_f = 1 \) as

\[
z(x, y) = \sum_{k=0}^{N} \frac{(N-k)!}{N!k!} (M(x)M(y))^k + \kappa \left((-1)^N \bar{B}(y)B(x) + \bar{B}(x)B(y)\right).
\]

(3.2.16)

If we include an anisotropic coupling \( \gamma \) and a chemical potential \( \mu \) in \( S_F \), additional prefactors appear. In this case, the one-link integral reads [9]

\[
z(x, y) = \sum_{k=0}^{N} \frac{(N-k)!}{N!k!} \left(\left(\eta_\mu(x)\gamma_{A_{4,\mu}}\right)^2 M(x)M(y)\right)^k
\]

\[
+ \kappa \left(\rho(y, x)^N \bar{B}(y)B(x) + \rho(x, y)^N \bar{B}(x)B(y)\right),
\]

\[
\rho(x, y) = \eta_{y-x}(x) \begin{cases} \gamma \exp(\pm a_\mu \mu) & \text{if } (y, x)_4 = \pm 1 \\ 1 & \text{else} \end{cases}
\]

(3.2.17)

(3.2.18)
3 The dual representation of SC-LQCD

3.3 Dual representation

As we have finished calculating the one-link integral, we can now use it to rewrite the partition sum $Z$ in terms of new degrees of freedom. We continue from (3.2.1) by plugging in our new result (3.2.17). In the remaining Grassmann integral, we face expressions of the form

$$\int d\chi(n) d\bar{\chi}(n) e^{2am\bar{\chi}(n)\chi(n)} (\bar{\chi}(n)\chi(n))^k.$$

These type of integrals can be carried out by using (A.2.7) and (A.3.2), yielding

$$\int d\chi(n) d\bar{\chi}(n) e^{2am\bar{\chi}(n)\chi(n)} (\bar{\chi}(n)\chi(n))^k = \int d\chi(n) d\bar{\chi}(n) \sum_{j=0}^{N} \frac{1}{j!} (2am\bar{\chi}(n)\chi(n))^j (\bar{\chi}(n)\chi(n))^k = \sum_{j=0}^{N-k} \frac{1}{j!} (2am)^j (\bar{\chi}(n)\chi(n))^j = \frac{N!}{(N-k)!} (2am)^{N-k}.$$

When taking the product over all lattice sites $n$ and all directions $\mu$, the Grassmann property (A.2.1) reduces the contributions to $Z$ to three types of objects: monomers, dimers and baryon-loops.

- The monomers $M(x)^{\bar{n}}$, $\bar{n}_n = 0, 1, \ldots, N$ are defined on the lattice sites and are generated by the mass term $e^{2am\bar{\chi}\chi}$.
- The dimers appear as non-oriented meson hoppings $(M(n)M(n \pm \hat{\mu}))^{k_n}$ which are defined on the bonds $b \in B(\Lambda)$ connecting the lattice sites. They define the bond occupation number $k_b = 0, 1, \ldots, N$.
- The baryon-loops $\bar{B}(n \pm \hat{\mu})B(n)$ form oriented, self-avoiding loops $l \subset B(\Lambda)$ on the bonds. We can define a baryonic bond variable $b_{\mu}(n)$ at each lattice site $n$ such that $b_{\mu}(n) = -1$ if the baryon link in $\mu$-direction is incoming, $b_{\mu}(n) = 0$ if the link is not occupied and $b_{\mu}(n) = 1$ if the baryon link is outgoing.

In Fig. 2 we give a graphical representation of these three objects.

![Figure 2: Graphical notation of dimers, monomers and baryons for SU(3).]
3.4 Energy density

The new degrees of freedom are accompanied by the constraints

\[ \tilde{n}_n + \sum_{\hat{\mu}=\pm 1, \pm 2, \ldots, \pm d} k_{(n, \hat{\mu})} = N \]  \hspace{1cm} (3.3.1)

\[ \sum_{\hat{\mu}=\pm 1, \pm 2, \ldots, \pm d} b_\mu(n) = 0. \]  \hspace{1cm} (3.3.2)

Additionally, baryonic links and mesonic d.o.f’s are not allowed to touch. This is due to the fact that \( B(x) \) already contains all available \( \chi_i \)’s. An example of a configuration, fulfilling the above constraints, is given in Fig. 3.

Summing over all such configurations \( \{ k, \tilde{n}, l \} \), the partition sum of one-flavor lattice QCD at strong coupling reads

\[ Z = \sum_{\{ k, \tilde{n}, l \} \in B(\Lambda)} \prod_{b \in B(\Lambda)} \frac{(N - k_b)!}{N! k_b!} \gamma^{\mu_1, \mu_2} \prod_{n \in \Lambda} N! (2am)^{\tilde{n}_n} \prod_{l \in B(\Lambda)} \omega(l), \]  \hspace{1cm} (3.3.3)

with the baryon weight

\[ \omega(l) = \frac{1}{\prod_{n \in l} N!} \sigma(l) \gamma^{N - N_\hat{\gamma}} \exp(N \cdot N_r a \gamma \mu), \]  \hspace{1cm} (3.3.4)

and the sign

\[ \sigma(l) = (-1)^{r_\gamma + N_\hat{\gamma}(l) + 1} \prod_{b \in l} \eta_\mu(n). \]  \hspace{1cm} (3.3.5)

Here \( r_\gamma \) is the baryon loops winding number in temporal direction, \( N_\hat{\gamma} \) is the total number of baryonic links in temporal direction and \( N_\hat{\gamma}(l) \) is the total number of baryonic links in negative directions. The terms in (3.3.3) can be identified with the three types of contributions. The first term accounts for dimers, the second for monomers and the third for baryon loops.

3.4 Energy density

With \( Z \) written in terms of monomers, dimers and baryon loops, we can now derive an expression for the energy density in these new variables. Starting from the definition

\[ a^3 \epsilon = - \frac{1}{N^3} \frac{\partial}{\partial \beta} \log Z \bigg|_{a \gamma \mu}, \]  \hspace{1cm} (3.4.1)

we use \( \beta = \frac{1}{T} = N_r a \gamma \) and \( \xi(\gamma) = \frac{a}{a \gamma} \) to rewrite the derivative

\[
\begin{align*}
    a^3 \epsilon &= - \frac{1}{N^3} \frac{\partial}{\partial \beta} \log Z \bigg|_{a \gamma \mu} \\
    &= - \frac{1}{N^3 N_r} \frac{\partial}{\partial a \gamma} \log Z \bigg|_{a \gamma \mu} \\
    &= - \frac{1}{|\Lambda|} \left( \frac{\partial}{\partial h(\gamma)} \right) \log Z \bigg|_{a \gamma \mu}
\end{align*}
\]

\[
\begin{align*}
    &= - \frac{1}{|\Lambda|} \frac{1}{a} \left( \partial_{\gamma} \frac{1}{\Gamma(\gamma)} \right) \frac{\partial}{\partial \gamma} \log Z \bigg|_{a \gamma \mu} \\
    &= - \frac{1}{|\Lambda|} \frac{1}{a} \frac{\partial}{\partial h(\gamma)} \frac{\partial}{\partial \gamma} \log Z \bigg|_{a \gamma \mu},
\end{align*}
\]

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where we defined the function $h(\gamma) = \frac{1}{\xi(\gamma)}$ in the last line. Application of the chain rule to the logarithm yields

$$\frac{\partial}{\partial \gamma} \log Z \bigg|_{a_\tau \mu} = \frac{1}{Z} \frac{\partial Z}{\partial \gamma} \bigg|_{a_\tau \mu}.$$  

We now abbreviate the three terms of $Z$ according to their type of contribution

$$Z = \sum_{\{k, \vec{n}, l\}} DMB$$

and note that

$$\frac{\partial Z}{\partial \gamma} \bigg|_{a_\tau \mu} = \sum_{\{k, \vec{n}, l\}} \frac{\partial D}{\partial \gamma} \bigg|_{a_\tau \mu} MB + DM \frac{\partial B}{\partial \gamma} \bigg|_{a_\tau \mu},$$

since the monomer contribution $M$ is independent of the anisotropy $\gamma$. For the dimer term, we enumerate the bonds such that

$$\frac{\partial D}{\partial \gamma} \bigg|_{a_\tau \mu} = \frac{\partial}{\partial \gamma} \prod_{b \in B(\Lambda)} \frac{(N - k_b)!}{N! k_b!} \gamma^{2 k_b} = \delta_{1,\mu} 2 k_{b_1} \gamma^{2 k_b} W(b_1) \prod_{b \neq b_1} W(b) \gamma^{2 k_b} + \ldots$$

Contrary to what this notation might suggest, these different contributions are not independent. They strongly depend on each other through the constraints (3.3.1) and (3.3.2).
Here we defined $W(b) = \frac{(N-k_b)!}{N!k_b!}$ for readability. Note that the derivative reproduced the factors excluded in the products. Thus we can write

$$\left. \frac{\partial D}{\partial \gamma} \right|_{a_\tau \mu} = \left( \sum_b \frac{1}{\gamma} \delta_{4,\mu} 2k_b \right) \prod_b W(b) \gamma^{\delta_{4,\mu} 2k_b} = \frac{1}{\gamma} 2N_{D_t} \cdot D,$$

where $N_{D_t}$ is the number of dimers pointing in temporal direction.

Repeating this process for the baryonic term leads to

$$\left. \frac{\partial B}{\partial \gamma} \right|_{a_\tau \mu} = \left. \frac{\partial}{\partial \gamma} \prod_l \frac{1}{\prod_{x \in l} N!} \sigma(l) \gamma^{2} N_{N_4} \exp (N \cdot r_{l} a_\tau \mu) \right|_{a_\tau \mu} \left. \prod_l \omega(l) = \frac{1}{\gamma} N \cdot N_{B_t} B, \right.$$  

where $N_{B_t}$ denotes the number of baryonic bonds pointing in positive or negative temporal direction. Combining our results, we find

$$\left. \frac{\partial}{\partial \gamma} \log Z \right|_{a_\tau \mu} = \frac{1}{Z} \sum_{\{k,\bar{n},l\}} \frac{1}{\gamma} \langle 2N_{D_t} + N \cdot N_{B_t} \rangle DMB = \frac{1}{\gamma} \langle 2N_{D_t} + N \cdot N_{B_t} \rangle.$$

The energy density expressed in our dual variables therefore reads

$$a^4 \epsilon = -\frac{1}{|\Lambda|} \frac{1}{\gamma} \left. \frac{\partial}{\partial \gamma} \right(2N_{D_t} + N \cdot N_{B_t}) \right). \tag{3.4.2}$$

This concludes the discussion of the theoretical background and we move on to the numerical methods.
4 Methods

4.1 Monte Carlo method

After integrating out both gauge and quark degrees of freedom in (3.2.1), we obtained the partition sum

\[ Z = \sum_{\{k, \bar{n}, l\}} DMB, \]

as a sum over all configurations \( \{k, \bar{n}, l\} \) that fulfill the constraints (3.3.1) and (3.3.2). Expectation values of observables are then given by

\[ \langle O \rangle = \frac{1}{Z} \sum_{\{k, \bar{n}, l\}} O[k, \bar{n}, l] DMB. \] (4.1.1)

Analytic calculations of such sums are only possible for very small lattices because the number of configurations grows drastically with increasing lattice size. Therefore, we will use a statistical method, the Monte Carlo method, to evaluate such expressions. The main idea of the Monte Carlo method is to approximate the exact mean value (4.1.1) by a sample mean

\[ \langle O \rangle_S = \frac{1}{N} \sum_{i=1}^{N} O_i, \] (4.1.2)

where the observable \( O \) is evaluated on \( N \) randomly generated configurations. It can be shown that the error of this approximation is of the order \( O \left( \frac{1}{\sqrt{N}} \right) \) if the \( N \) measurements are statistically independent [8].

According to (2.6.7), the field configurations follow the Boltzmann distribution \( e^{-SE} \). In order to yield a useful estimate of the exact mean, the algorithm that generates the sample configurations has to draw them such that they approximate this Boltzmann distribution. This is called importance sampling [7].

4.2 Markov chains

Algorithms that generate such random configurations are usually implemented as Markov Chains. Starting from some initial configuration \( C \), a new configuration \( C' \) is generated by applying random changes to \( C \), following a probability distribution \( P(C) \). Successive updates create a chain of configurations

\[ C_1 \rightarrow C_2 \rightarrow \cdots \rightarrow C_N, \]

where each \( C_i \) only depends on \( C_{i-1} \). This last statement, the Markov property, is the defining feature of a Markov chain. The transition matrix elements \( T_{ij} = P(C_i|C_j) \) are normalized such that

\[ \sum_i T_{ij} = 1, \] (4.2.1)
indicating that there is always a transition from $C_j$ to any other configuration, including $C_j$ itself.

An important property of a Monte Carlo algorithm is ergodicity:

$$\exists n \in \mathbb{N} : (T^n)_{ij} > 0 \ \forall i, j.$$  \hspace{1cm} (4.2.2)

Starting from an arbitrary configuration, an ergodic algorithm can reach any other configuration of the configuration space in a finite number of steps. Non-ergodic algorithms, however, can be restricted to only a limited subspace of the configuration space which leads to wrong results.

For a given initial configuration with an initial distribution $P(C)_0$, we expect that successive updates lead the system towards the equilibrium distribution $P(C)_{eq}$

$$\lim_{n \to \infty} T^n P_0 = P_{eq}. \hspace{1cm} (4.2.3)$$

This implies that the equilibrium distribution is a fixed point of the Markov chain [7]

$$TP_{eq} = P_{eq}. \hspace{1cm} (4.2.4)$$

A sufficient condition for (4.2.4) is given by the detailed balance condition

$$T_{ji} P(C_i)_{eq} = T_{ij} P(C_j)_{eq}. \hspace{1cm} (4.2.5)$$

### 4.3 Worm algorithm

To generate configurations $\{k, \bar{n}, l\}$ that fulfill the constraints (3.3.1) and (3.3.2), we will use the **Worm algorithm**, an extension of the directed path algorithm developed in [4]. It consists of three parts, a mesonic worm update, a baryonic worm update and a monomer update. Each of these parts fulfills detailed balance as required in the previous subsection and the full algorithm is ergodic.

At first, we split our lattice in active and passive sites and split our partition sum into products over active and passive site weights (see [9])

$$Z = \sum_{\{k, \bar{n}, l\}} \prod_{x_a} W_a(x_a) \prod_{x_p} W_p(x_p) \sigma(\{k, \bar{n}, l\}), \hspace{1cm} (4.3.1)$$

with

$$W_a(x) = \prod_{\hat{\nu} = \pm 1, \ldots, \pm d} \left( \frac{(N - k_{(x, \hat{\nu})})!}{N! k_{(x, \hat{\nu})}!} \exp \left( 3b_{\hat{\nu}}(\delta_{\hat{\nu} \hat{\nu}} + \delta_{\hat{\nu} - \hat{\nu}})a_{\tau \mu} \right) \right) \frac{N!}{n_x!} (2am)^{n_x} \hspace{1cm} (4.3.2)$$

$$W_p(x) = \prod_{\hat{\nu} = \pm d} \left( \gamma^{2k_{(x, \hat{\nu})} + 3|b_{\hat{\nu}}|} \right) \frac{N!}{n_x!} (2am)^{n_x}. \hspace{1cm} (4.3.3)$$

The mesonic update consists of three steps:
4 Methods

1. A site $x$ that is not traversed by a baryonic sequence is drawn with uniform probability. This site now defines the set of active sites $x_a$. These are all sites with parity $\epsilon(x) = (-1)^{\sum x_i}$. This step is accepted with probability

$$P_x = \frac{N - n_x}{N}.$$ 

The monomer number $n_x$ is then increased by one and a direction $\hat{\mu}$ is chosen with probability

$$P_{\hat{\mu}} = \frac{k_{(x,\hat{\mu})}}{N}.$$ 

The dimer number in this direction is reduced by one and the total change at $x$ is $(n_x \to n_x + 1, k_{(x,\hat{\mu})} \to k_{(x,\hat{\mu})} - 1)$.

2. The worm’s head is now located at the passive site $y = x + \hat{\mu}$. From here, a new direction $\hat{\rho}$ is chosen with a so-called heat-bath probability

$$P_{\hat{\rho}} = \frac{W_{\hat{\rho}}(y)}{W_D(y)}, \quad W_D(y) = \sum_{\hat{\nu}} W_{\hat{\nu}}(y),$$

where the weights are given by

$$W_{\hat{\nu}}(y) = \begin{cases} \gamma^{2k_{(y,\hat{\nu})}} & \text{if } b_{(y,\hat{\nu})} = 0 \\ 0 & \text{if } b_{(y,\hat{\nu})} \neq 0. \end{cases}$$

The link occupation number in this direction is then incremented by one: $(k_{(y,\hat{\rho})} \to k_{(y,\hat{\rho})} + 1)$.

3. We continue by moving to the next site $z = y + \hat{\rho}$. This site is active again and we have two options:

   a) We either choose another direction $\hat{\nu} \neq -\hat{\rho}$, continue the worm by deleting a dimer in $\hat{\nu}$-direction and repeat step 2,
   b) or, provided that $n_z \neq 0$, we delete a monomer at $z$ and close the worm update.

The probability to end the update is given by

$$P_z = \frac{n_z}{N - k_{(z,\hat{\rho})}},$$

while the direction $\hat{\nu}$ is accepted with probability

$$P_{\hat{\nu}} = \frac{k_{(z,\hat{\nu})}}{N - k_{(z,\hat{\rho})}}.$$
Note that in the chiral limit $m_q = 0$ the update can only close if the worm head returns to the starting position since this is the only site containing a monomer. It is also possible to allow backtracking in step 3a). This leads to the *diffusive worm algorithm*.

An example of a full mesonic update is shown in Fig. 4. Going from configuration (a) to (b), the site (3,2) is chosen to be the update’s starting point and a monomer is added. The dimer on the bond left to (3,2) is deleted. Following step 2 in (c), a dimer is added between (2,2) and (2,1). As there is no monomer at (2,1), the update has to continue by choosing another direction and deleting a dimer on the corresponding link. After another repetition of steps 2 and 3, the update ends at configuration (f) by deleting the monomer that was introduced in step 1.

![Figure 4: A complete mesonic worm update. The blue (red) monomer indicates the position of the worm’s head (tail).](image)

Similar to the mesonic update, the baryonic worm update consists of active and passive steps.

1. With uniform probability, we draw a site $x$ that is either part of a baryon-loop or touched by an $N$-dimer.
   
   a) If $x$ is a baryonic site, we proceed in negative flux direction by deleting the baryon on that link.
   
   b) If $x$ is touched by a $N$-dimer, we convert this $N$-dimer into an outgoing baryonic segment.

2. Moving on to site $y = x + \hat{\mu}$, we choose an outgoing direction $\hat{\rho}$ with the heat-bath probability (4.3.4) using the weight

$$W_{\hat{\rho}}(y) = \gamma^{3\delta_{\hat{\rho},\pm4}} \exp \left( 3a_+ \mu (\delta_{\hat{\rho},4} + \delta_{\hat{\rho},-4}) \right)$$
4 Methods

if $y + \hat{\rho}$ is part of a baryon or touched by an $N$-dimer and $W_{\rho}(y) = 0$ else. If $y + \hat{\rho}$ is a mesonic site, we replace the corresponding 0-dimer or $N$-dimer by a positive baryon flux. Otherwise, we either remove or produce a baryonic link depending on whether or not the link in $\rho$-direction is occupied by a baryon.

3. If the active site $z = y + \hat{\rho}$ happens to be the site from which the worm evolution started, the update ends. Otherwise, $z$ is either traversed by a baryon or touched by an $N$-dimer such that we continue with step 1a) or 1b).

The monomer update can be realized by local algorithms like the Metropolis algorithm. The update relies on replacing a dimer by two monomers and vice versa. Such a replacement is sketched in Fig. 5. As monomers are absent in the chiral limit, where our simulations are performed, we do not go into further detail here.

![Figure 5: Local monomer update.](image)

4.4 Jackknife

The Jackknife method is used to obtain an estimate of the variance of an observable $x$ on a given set of data. The sample, consisting of $n$ data points $x_1, x_2, \ldots, x_n$, is divided into $N$ subsets of size $M$. $N$ new subsets are constructed by omitting the $i$'th subset from the original sample. On these reduced samples, new estimators $\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_N$ are calculated. Their mean

$$\tilde{x} = \frac{1}{N} \sum_{i=1}^{N} \hat{x}_i \quad (4.4.1)$$

can be used to calculate the bias as

$$B = (N - 1)(\tilde{x} - \hat{x}). \quad (4.4.2)$$

Here, $\hat{x}$ denotes the estimator of $x$ on the original sample. The bias-corrected Jackknife estimator is then

$$\hat{J} = \hat{x} - B = N\hat{x} - (N - 1)\tilde{x} \equiv \frac{1}{N} \sum_{i=1}^{N} \hat{J}_i. \quad (4.4.3)$$

The last expression defines the Jackknife pseudo values

$$\hat{J}_i = N\hat{x} - (N - 1)\hat{x}_i. \quad (4.4.4)$$

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They are interpreted as bias-corrected, independent data points such that the variance of their mean is given by

\[
\sigma_J^2 = \frac{1}{N(N-1)} \sum_{i=1}^{N} (\hat{J}_i - \hat{j})^2
\]

\[
= \frac{1}{N(N-1)} \sum_{i=1}^{N} (N\hat{x} - (N-1)\hat{x}_i - N\hat{x} + (N-1)\bar{x})^2
\]

\[
= \frac{N - 1}{N} \sum_{i=1}^{N} (\hat{x}_i - \bar{x})^2. \tag{4.4.5}
\]

In our simulation, successively generated data points are not independent so the empirical variance is not reliable. Therefore, (4.4.5) will serve as an estimate of the variance of \( \hat{x} \).
5 Nuclear physics at strong coupling

5.1 Baryon mass

An important parameter entering the calculation of the nuclear potential is the baryon mass $m_B$. The strategy to calculate it is to simulate two systems, one containing a static baryon, represented by a baryonic loop in purely temporal direction (see Fig. 3) that is excluded from the updating process, and one without such. As the baryon’s kinetic energy is zero, the change in energy $\Delta E$ between those two systems is the baryon mass $m_B$. To estimate $\Delta E$, two different approaches are used in this thesis, the snake algorithm and a direct method based on (3.4.2). Both will also be used to calculate the nuclear potential later on.

Snake algorithm

Since the free energy $F$ is related to the energy $E$ by the Legendre transformation

$$F = E - TS,$$  \hspace{1cm} (5.1.1)

$E$ can be approximated by $F$ at low temperature. Furthermore, $F$ is related to the partition sum by

$$F = -T \log Z,$$  \hspace{1cm} (5.1.2)

which implies that the difference in free energy between two systems is

$$\Delta F = F_1 - F_2 = -T (\log Z_1 - \log Z_2) = -T \log \frac{Z_1}{Z_2}. \hspace{1cm} (5.1.3)$$

If we denote by $Z_{N_\tau}$ the partition sum of the system containing a static baryon of length $N_\tau$ and by $Z_0$ the partition sum of the free system, we can use (5.1.3) to approximate the energy difference between these two systems

$$\Delta E \approx \Delta F = - T \log \frac{Z_{N_\tau}}{Z_0}.$$  

By computing the ratio $\frac{Z_{N_\tau}}{Z_0}$ via Monte Carlo simulations, we can then extract the baryon mass. However, the probability to have a full static baryon on the lattice

$$\frac{Z_{N_\tau}}{Z_0} = \exp \left( - \frac{\Delta F}{T} \right) \approx \exp \left( - \frac{m_B}{T} \right) = \exp (-aN_\tau m_B) \hspace{1cm} (5.1.4)$$

is of the order $O(10^{-11})$ if we assume the mean field value $m_B \approx 3$ and $N_\tau = 8$ [9]. Obtaining a reliable result for $m_B$ from this ratio is therefore impossible. To circumvent this, we factorize

$$\frac{Z_{N_\tau}}{Z_0} = \frac{Z_{N_\tau}}{Z_{N_\tau - 2}} \frac{Z_{N_\tau - 2}}{Z_{N_\tau - 4}} \ldots \frac{Z_2}{Z_0} \hspace{1cm} (5.1.5)$$
and calculate each of these ratios with Monte Carlo simulations. To do so, we have to replace the baryon loop by a sequence of $0 - N$ dimers as shown in Fig 6. This is possible since both objects carry exactly the same weight at $\mu = 0$ which can be seen in (3.3.3) and (3.3.4). In the actual simulation, the volume corresponding to a sequence of $0 - N$ dimers of length $l - 2$ is excluded from the worm updates and the $N$-dimer occupation rate of the subsequent temporal link is measured. In this way, we obtain $Z_l / Z_{l-2}$. The baryon mass is then given by the sum

$$am_B = -\frac{1}{N_\tau} \left( \log \left( \frac{Z_{N_r}}{Z_{N_r-2}} \right) + \log \left( \frac{Z_{N_r-2}}{Z_{N_r-4}} \right) + \cdots + \log \left( \frac{Z_{2}}{Z_{0}} \right) \right).$$

(5.1.6)

Alternatively, we can plot these ratios as a function of $l$. Apart from finite size effects at the boundaries, they form a plateau which can be fitted. The sum in (5.1.6) can then be replaced with $-\frac{1}{2} \log \left( \frac{Z_{l+2}}{Z_l} \right)$.

Figure 6: Replacement of a baryon loop by a sequence of 0 and triple dimers.

Figure 7: $\frac{Z_l}{Z_{l-2}}$ as a function of $l$ for $U(3)$ on a $10^4$ lattice.
with $\frac{N_t}{2} \log \left( \left\langle \frac{Z_l}{Z_{l-2}} \right\rangle \right)$ since there are $\frac{N_t}{2}$ terms in the sum. The baryon mass is then given by

$$am_B = -\frac{1}{N_t} \frac{N_t}{2} \log \left( \left\langle \frac{Z_l}{Z_{l-2}} \right\rangle \right) = -\frac{1}{2} \log \left( \left\langle \frac{Z_l}{Z_{l-2}} \right\rangle \right),$$

(5.1.7)

where $\log \left( \left\langle \frac{Z_l}{Z_{l-2}} \right\rangle \right)$ is the value obtained from the fit. An example for such a plateau is shown in Fig. 7 for a $10^4$ lattice. Other examples can be found in [9], where similar calculations were performed on a $8^3 \times 16$ lattice. While this procedure is quite effective for large $N_t$, it becomes unreliable at smaller lattice sizes as there are not enough ratios to form a plateau. All our simulations are performed on such small lattices so we will use (5.1.6) directly to calculate $am_B$. 

5.1 Baryon mass

Direct method

An alternative way to obtain the difference in energy is to calculate it directly by using (3.4.2)

\[ aE = N^3 a^4 \epsilon = -\frac{1}{N} \frac{\partial \gamma}{\partial h(\gamma)} \langle 2N_D t + N \cdot N_B t \rangle, \quad h(\gamma) = \frac{1}{\xi(\gamma)}. \]

The values of \( N_t, N_\sigma, N \) and \( \gamma \) are input parameters of the simulation, whereas \( \langle N_D t \rangle \) and \( \langle N_B t \rangle \) are determined during it. The derivative \( \frac{\partial \gamma}{\partial h(\gamma)} \), on the other hand, is obtained in a more demanding way. It relies on the knowledge of the dependence of the anisotropic coupling \( \gamma \) on the physical anisotropy \( \xi \). \( \gamma(\xi) \) can be measured by another type of Monte Carlo simulations. The concept of these simulations is sketched at the end of section 5.3. They were performed by Dr. Wolfgang Unger who also provided an analytic Ansatz for \( \gamma \). The result is shown in Fig. 8.

![Figure 8](image)

**Figure 8:** The anisotropic coupling plotted against \( \xi \). The red curve is an analytic Ansatz for \( \gamma(\xi) \). The blue line is the slope of this Ansatz at \( \xi = \frac{a}{a_t} = 1 \).

Following the strategy described in the beginning of this chapter, we obtain \( m_B \) by performing two simulations, one with a static baryon which is excluded from the worm updates and one without this constraint.
5 Nuclear physics at strong coupling

Results

We calculated the baryon mass for both gauge groups \( U(3) \) and \( SU(3) \) on a \( 3+1 \) dimensional hypercubic lattice with \( N_\tau = N_\sigma = 8 \). The simulations were performed in the chiral limit, \( m_q = 0 \), and at \( \gamma = 1 \). The results are listed in Tab. 1. The difference between the \( U(3) \) and \( SU(3) \) results obtained by the snake algorithm are very small due to the strong suppression of baryon loops at low temperature and both are relatively close to the mean-field value of \( am_B = \text{asinh} \left( \frac{1}{2} (2d)^{N/2} (1 - \frac{N}{d}) \right) \approx 2.914 \). The direct method, on the other hand, yields a much lower value for the baryon mass. This raises the question of whether the snake- or the direct method is more reliable.

In (5.1.4), we approximated \( \Delta F = \Delta E - T \Delta S \approx \Delta E \), which scales linearly with \( T \). Therefore, we expect to see a linear decrease of \( m_{B,\text{snake}} \) towards \( m_{B,\text{direct}} \) for increasing \( N_\tau \). To get a better understanding of the influence of finite size and temperature effects on \( m_B \), we also calculate the mass for all combinations of \( N_3 \cdot N_\tau \) with \( N_\sigma, N_\tau = 4, 6, 8, 10 \). The simulations are performed for the \( U(3) \)-theory only as the difference to \( SU(3) \) is very small and \( SU(3) \) simulations demand a much greater numerical effort.

Table 1: The baryon mass \( am_B \) on \( 8^4 \) lattices.

<table>
<thead>
<tr>
<th>Method</th>
<th>( U(3) )</th>
<th>( SU(3) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Snake</td>
<td>2.879(1)</td>
<td>2.877(2)</td>
</tr>
<tr>
<td>Direct</td>
<td>2.146(2)</td>
<td>-</td>
</tr>
<tr>
<td>Mean-field</td>
<td>-</td>
<td>2.914</td>
</tr>
</tbody>
</table>

The dependence of the mass on finite size effects for various temperatures is shown in Fig. 9. There, we also try to extrapolate the results to \( N_3^2 \to \infty \) by fitting the data with a linear Ansatz. The values with \( N_\sigma = 4 \) are excluded from the fit because the effects of the boundary conditions on such small lattices are very large. The extrapolated values are plotted against their corresponding temperature in Fig. 10. Unfortunately, the errors on these extrapolated masses are too large to allow for a meaningful extrapolation towards \( T = 0 \). Instead, we can try to extrapolate simultaneously \( N_\sigma = N_\tau \to \infty \), which is done in Fig. 11. Within the reached precision, the linear Ansatz matches the results quite well and we obtain for the extrapolated mass at \( T = 0 \): \( am_{B,\text{ext}} = 2.8785(7) \). While this value is close to the ones that were obtained by the snake algorithm on \( 8^4 \) lattices, it is still far away from \( m_{B,\text{direct}} \) and no sign of convergence towards this method is found.

The same calculations are performed with the direct method and the results are shown in Fig. 12. Here, we see that none of the above extrapolations can be repeated for these data. No clear trend can be read off from these results so we stick to the value in Tab. 1 and conclude that the different methods do not agree, not even in the limit \( N_\sigma = N_\tau \to \infty \). We will encounter this problem again and discuss it in further detail when we calculate the nuclear potential in section 5.3.

\[ ^4 \text{As seen during the calculation of the one-link integral, there are no baryons in the U(3) theory. However, we can still exclude the volume corresponding to a} \: 0 - N \: \text{dimer sequence from the updating process.} \]
5.1 Baryon mass

Figure 9: $am_B$ for various lattice sizes.

Figure 10: Extrapolated masses.
Figure 11: Simultaneous extrapolation $N_\tau = N_\sigma \to \infty$.

Figure 12: $am_B$ calculated with the direct method.
5.2 Meson cloud

Adding a static baryon to the lattice has another effect apart from raising the system’s energy by $am_B$. As we shall see soon, the energy density of the surrounding meson cloud is modified as well. In absence of baryons and at $m_q = 0$, $\gamma = 1$, the probability to have a dimer pointing in temporal direction is given by $\langle k_{n,d} \rangle = \frac{N}{2d}$ because there are $N$ dimers connected to site $n$ and $2d$ adjacent bonds that can be occupied. This probability is changed in direct neighborhood of a static baryon. Since mesonic degrees of freedom and baryonic loops are not allowed to touch at $N_f = 1$, the bond connecting the site $n$ with a static baryon at $n + \hat{\nu}$ cannot be occupied so the number of available spatial bonds is lowered and $\langle k_{n,d} \rangle$ is increased. Similarly, the sites with distance $r/a = \sqrt{2}$ to the static baryon will have an energy density lower than $\frac{N}{2d}$ because their bond occupation numbers pointing towards the baryon’s nearest neighbors are increased. While this oscillation continues, the amplitude will decrease with increasing distance $r$. We can quantify this effect by using (3.4.2) to define the change in energy density

$$a^4 \delta \epsilon (r) := -\frac{1}{\gamma \partial h(\gamma)} \langle 2n_{D_t}(r) + N \cdot n_{B_t}(r) \rangle - \epsilon_{vac},$$

(5.2.1)

where

$$n_{D_t}(r) = \frac{N_{D_t}(r)}{N_t \cdot N(r)}, \quad n_{B_t}(r) = \frac{N_{B_t}(r)}{N_t \cdot N(r)}.$$ 

Here, $N_{D_t}(r)$ is the number of temporal dimers and $N(r)$ is the number of spatial lattice sites at distance $r$ from the static baryon. $N_{B_t}(r)$ is the total number of baryons and anti-baryons in temporal direction at distance $r$ and $\epsilon_{vac}$ is the energy density of the free system. We calculate this change in energy density on a $16^4$ lattice with gauge group $U(3)$. The result is shown in Fig. 13. The expected oscillatory behavior as well as the amplitude’s damping is captured well by the data. Taking a closer look at the sign of $\delta \epsilon$, we find that it is given by $(-1)^{n_1 + n_2 + n_3 + 1}$.

![Figure 13: $\delta \epsilon (r)$ for $U(3)$ on a $16^4$ lattice.](image)
5 Nuclear physics at strong coupling

By plotting the absolute value of $\delta \epsilon$ on a logarithmic scale, an exponential decay can be seen. In the continuum, such a disturbance in the meson cloud’s energy is described by a profile of Yukawa form

$$V_{\text{Yukawa}}(r) \propto -\frac{e^{-mr}}{r},$$

where $m$ is the mass of the meson. It is obtained by Fourier-transformation of the free boson propagator

$$\int \frac{d^3k}{(2\pi)^3} \frac{e^{ikr}}{k^2 + m^2} = \frac{e^{-mr}}{4\pi r}.$$ 

To describe the lattice data, we compute the discrete free boson propagator $K \left( \frac{r}{a} = |i - j| \right) = A(D^{-1})_{ij}$ by inverting the Dirac operator

$$D_{ij} = \frac{1}{2} \left( ((am)^2 + 2d) \delta_{ij} - \sum_{\mu=1}^d (\delta_{i-\hat{\mu},j} + \delta_{i+\hat{\mu},j}) \right)$$

on a $16^3$ lattice. After computing $K \left( \frac{r}{a} \right)$ for various masses, we can fit the propagator to $a^4|\delta \epsilon|$, using $m$ and $A$ as fitting parameters.

![Figure 14: $|\delta \epsilon(r)|$ for $U(3)$ and the free boson propagator on a $16^4$ lattice.](image)

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The resulting parameters are $A = 27.7(1)$ and $m = 1.94(2)$. The fit plotted in Fig. 14 is in excellent agreement with the Monte Carlo data at small distances. At larger distances, the obtained accuracy is too low to capture the exact behavior of $K(x)$. Up to effects stemming from the lattice discretization, the meson cloud’s energy profile is

$$
\delta \epsilon (r) \sim -\frac{e^{-mr}}{r} (-1)^{n_1+n_2+n_3}.
$$

(5.2.4)

The phase $(-1)^{n_1+n_2+n_3}$ characterizes the $\rho$-meson in the staggered formulation (see section 4.1.3 of [9]) and the fit parameter $m$ is related to the mass of the $\rho$-meson by

$$
am_{\rho} = \cosh \left( 1 + \frac{(am)^2}{2} \right).
$$

(5.2.5)

From this equation, we obtain $am_{\rho} = 1.72(2)$ which is close to the mean field value $am_{\rho,\text{M.F.}} = 1.76$ [13].

The influence of a static baryon also has an interesting physical consequence. By disturbing the meson cloud, the former point-like baryon obtains an extended shape and becomes a macroscopic object.
5 Nuclear physics at strong coupling

5.3 Nuclear potential

Now that we studied the effects of a single static baryon on the lattice, we can investigate how the system changes when a second baryon is added. In particular, this will enable us to study their interaction, giving rise to the nuclear potential $V_{NN}$. With two static baryons present on the lattice, two modified meson clouds are present as well. These two clouds can overlap and influence each other. Up to second order effects and at large distances, one can assume that they simply add up. Thus, we expect the potential to be given by

$$aV_{NN}(r) = a\Delta E - am_B \approx -2a^4\delta\epsilon(r).$$

(5.3.1)

This implies that the nuclear potential should be proportional to (5.2.2) as well. To check this hypothesis, we calculate $V_{NN}$ with both methods on a $8^4$ lattice at $m_q = 0$, $\gamma = 1$ and with $G = U(3)$. For each distance $r$ that we want to measure, we have to run a separate simulation. At those distances where there is more than one possible type of neighborhood relation, all possible geometries have to be simulated separately. For our chosen radii, this occurs only at $r/a = 3$. Up to permutations of indices, we can either place a baryon at $x = (2, 2, 1)$ or at $(3, 0, 0)$ to obtain this distance. However, these two lattice vectors have distinct neighborhood relations to the origin, where the other baryon is located, and yield different results.

In the case of the snake algorithm, the number of simulations is even greater. The procedure to calculate $\Delta F$ is almost the same as in section 5.1. The only difference here is that the site $x = (x_1, x_2, x_3)$ is occupied by a full static baryon. Each value calculated with the snake algorithm is obtained by $N_{\tau}/2$ simulations. The results of the simulations are shown in Fig. 15.

Qualitatively, both methods show a similar behavior. At $r/a = 1$, a strong nearest neighbor attraction is visible which is more pronounced in the snake data. One step further from the origin, at $r/a = \sqrt{2}$, the sign changes and the potential is repulsive. Here, the repulsion of the direct method is larger than that of the snake algorithm. This observation continues to larger distances so the amplitude of the values obtained by the direct method is always larger than that of the snake values. The signs oscillate and the amplitudes are damped similar to what we observed for $\delta\epsilon$. Up to a phase factor, both methods show a potential of Yukawa shape. This is a very interesting observation from the physical point of view. At $N_f = 1$, baryons and mesons are not allowed to touch and thus $NNN$ vertices are forbidden such that pion exchange is absent in our model. In the continuum, it is this pion exchange that gives rise to the Yukawa potential. On the lattice, we are able to obtain a Yukawa potential even without such a particle exchange. The origin of our potential is purely entropic, similar to the Casimir effect in the continuum.

To verify that our calculated potential matches the meson cloud’s energy density, we fit $V_{NN}(r)$ to the free boson propagator obtained by inversion of (5.2.3). The fit is plotted on a logarithmic scale in Fig. 16 and the resulting parameters are listed in Tab. 2.

---

5 The same splitting is present in $\delta\epsilon$ but there we chose to average over different geometries for algorithmic simplicity.
5.3 Nuclear potential

Table 2: Fit-parameters and $\rho$-mass for $V_{NN}$.

<table>
<thead>
<tr>
<th>Method</th>
<th>$A$</th>
<th>$am$</th>
<th>$am_\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct</td>
<td>28.6(7)</td>
<td>0.55(5)</td>
<td>0.54(4)</td>
</tr>
<tr>
<td>Snake</td>
<td>74.2(2)</td>
<td>1.83(3)</td>
<td>1.63(2)</td>
</tr>
</tbody>
</table>

Figure 15: $V_{NN}(r)$ for $U(3)$ on a $8^4$ lattice.

Figure 16: Free lattice boson propagator fitted to $V_{NN}(r)$. 
Before we discuss the direct method, we will analyze the results of the snake algorithm. The mass \( am_{\rho, S} = 1.63(2) \) is about 0.1a smaller than the value obtained from \( \delta \epsilon \). This mismatch is certainly larger than expected but it might be that with increasing statistics the difference could still shrink. Apart from the small \( \rho \)-mass, \( V_{NN}(r) \) is well described by the Yukawa potential up to distances of around \( r/a = 3.5 \). To see if the calculated potential is actually twice as large as \( \delta \epsilon \), we can fit the meson cloud’s energy directly to \( V_{NN}(r) \). The fit is shown in Fig. 17.

\[
\begin{align*}
\text{Snake} & \quad a \delta \epsilon, \ a=3.121 \\
\end{align*}
\]

**Figure 17:** Comparison between \( \delta \epsilon \) and \( V_{NN} \).

Both quantities match fine but the expectation that \( V_{NN} \approx -2 \delta \epsilon \) is not met. Instead, we find a factor of \( a = 3.12(4) \) which seems to disprove our hypothesis. We note that this proportionality factor crucially depends on the knowledge of the derivative \( \frac{\partial \gamma}{\partial h(\gamma)} \). In earlier works such as [9], the value of this derivative was unknown and it was found that \( a \approx 2.1 \) if the prefactor is omitted. We can check if our results match the earlier calculations by repeating the fit while setting \( \frac{\partial \gamma}{\partial h(\gamma)} \equiv 1 \). We find \( a|_{\gamma=1} = 2.19(3) \) which is in agreement with the earlier results. While these results may seem promising, one must not forget that a reliable prefactor can only be determined when \( \frac{\partial \gamma}{\partial h(\gamma)} \) is known. If we made no mistake concerning this derivative, higher order effects in the interaction of the meson clouds must have significant influence on the nuclear potential. Such effects, however, are likely to introduce a much more complex behavior and usually do not result in a simple constant. Therefore, we speculate that the mismatch might be due to a mistake connected to \( \frac{\partial \gamma}{\partial h(\gamma)} \). At this point, we do not have enough
5.3 Nuclear potential

Turning back to the fit in Fig. [16] we still have to analyze the results of the direct method. This method yields an even smaller $\rho$-mass of $m_{\rho,D} = 0.54(4)$. Compared to $V_{NN,S}(r)$ or $\delta\epsilon(r)$, this mass indicates a much slower exponential decay so a fit of $\delta\epsilon$ to $V_{NN,D}$ to obtain their proportionality factor as above is useless since their shapes are too different. Again, we face the problem that the direct method strongly disagrees with the results of the snake algorithm, while the latter enjoys a rather good accord to analytic predictions. Therefore, we conclude that there must be a severe error in the direct method itself.

The key ingredient to this method, and the reason why it was not available in earlier works, is the knowledge of the derivative $\frac{\partial \gamma}{\partial h}(\gamma)$. The calculation of this derivative relies on comparing conserved charges $j_\mu$ that are equal if the physical lattice is isotropic, that is $N_\tau a_\tau = N_\sigma a_\sigma$. These charges depend on the baryonic and mesonic occupation numbers $b(n,\nu)$, $k(n,\nu)$. The introduction of static baryons on the lattice disturbs those occupation numbers as we have seen in section 5.2. Therefore, the charges are changed in the presence of static baryons and we expect different derivatives compared to the free case. In the thermodynamic limit, the perturbations that enter the charges should vanish as their contribution to the average occupation numbers reduces with increasing lattice size. Our simulations, on the other hand, were all performed on rather small lattices so a significant contribution should be visible. So far, we did not take this consideration into account and we always used the derivative obtained on free lattices. Measuring the derivative of the anisotropic coupling in the presence of one baryon as well as the two baryon configurations used above might solve the problems we faced when applying some form of (3.4.2).

At last, we want to compare our results to the nuclear potential in the continuum. In Fig. [18] three examples of phenomenological nuclear potentials are shown. They all exhibit a hard-core repulsion at short ranges and a minimum at $r \approx 0.8$. In between $r = 1$ and $r = 2$, the potential is governed by heavy mesons such as $\rho$, $\omega$ and $\sigma$ and at distances larger than $r = 2$, it is described by pion exchange. The lattice results share some of these features as well. The hard-core repulsion is present in our model at $r = 0$ and arises trivially from the Grassmann constraint. It is followed by the already mentioned strong nearest neighbor attraction at $r = 1$ and we found that the data at $r \geq 1$ can be described by a discrete Yukawa potential. Up to the oscillating sign, this might be interpreted as an approximation of the second region of the continuum potential. The transition from the hard-core repulsion to the minimum is not resolved by our model and the pion exchange region is also missing. This might change if larger $N_f$ are considered or if simulations at $\beta > 0$ are performed.
5 Nuclear physics at strong coupling

Figure 18: Examples for nuclear potentials in the continuum \[14\].
6 Summary and outlook

In this thesis, we studied baryonic properties of one-flavor staggered fermions at strong coupling. For this purpose, we applied two techniques to calculate energy differences, the snake algorithm and a direct method based on the definition of energy. With these techniques, we were able to calculate the baryon mass $am_B$. While the snake algorithm provided a mass that was in good agreement with mean field predictions, the direct method yielded a significantly smaller mass. We speculated that these two methods might agree in the thermodynamic limit as $\Delta F$ is supposed to converge linearly towards $\Delta E$. The linear decrease we found was not steep enough to reach the value predicted by the direct method at $T = 0$. Thereafter, we investigated the influence of a baryon on the surrounding meson cloud. Up to a phase factor, we found that the energy density of the meson cloud can be described by the free boson propagator and its exponential decay is related to the $\rho$-mass. The resulting $\rho$-mass agreed well with the mean field results. We argued that the disturbed meson cloud extends the former point-like baryon to a macroscopic object with exponentially damped profile. By adding a second baryon to the lattice, we were able to calculate the nuclear potential. Both methods provided a potential that is of Yukawa shape. As there is no pion exchange at $N_f = 1$, the potential originates from an entropic effect similar to the Casimir effect. By fitting the calculated potentials to the free boson propagator, we saw that their exponential decay is substantially different. While the exponential decay of the snake method’s result is still somewhere in the vicinity of the $\delta \epsilon$ value, the direct method exhibits a much slower decay. By fitting $\delta \epsilon$ to the snake’s result, we were able to check if $V_{NN} \approx -2\delta \epsilon$. Instead of 2, we extracted the proportionality factor $a = 3.12(4)$. Lastly, we argued that the present mismatches might be due to the usage of the wrong value for $\frac{\partial \gamma}{\partial h(\gamma)}$. Unfortunately, the computational effort to determine those values for all the different baryon numbers and geometries is quite large and there was not enough time to compute these. It therefore remains an interesting question for future projects to determine the influence of static baryons on the anisotropic coupling $\gamma$. Further open questions concern the generalization of the dual representation to higher $N_f$. Monte Carlo simulations of lattice QCD at strong coupling with $N_f > 1$ have not been performed yet. In the view of the nuclear potential, it might be interesting to see how $V_{NN}$ changes with $N_f$ as it is conjectured that pion-exchange is possible at $N_f > 1$. Another aspect that was not studied in this thesis is the inclusion of $\beta$ corrections to the action. By so-called character expansions, it is possible to introduce gauge corrections to the dual representation that allow for simulations at $\beta > 0$. Although a lot of progress was made in this field within the last years, baryonic properties such as the nuclear potential at $\beta > 0$ have not been studied in the dual representation yet.
A Appendix

A.1 Haar measure

To include gauge fields into the lattice path integral, we have to find a suitable measure. This is done by defining the Haar measure $dU$, which is used to integrate over continuous compact groups [8]. It is normalized such that

$$\int_G dU = 1 \quad (A.1.1)$$

and it is invariant under right and left multiplication with group elements

$$dU = d(VU) = d(UV) \quad V \in G. \quad (A.1.2)$$

The latter also implies invariance under gauge transformations (2.3.6). For compact Lie groups, the group elements $U \in G$ can be expressed by a set of real variables $\omega_k$ by using the generators $T_k$

$$U = U(\omega) = \exp \left( i \sum_k \omega_k T_k \right).$$

With these $\omega_k$’s, one can define the measure $dU$ explicitly via

$$dU = c \sqrt{\det g(\omega)} \prod_k d\omega_k, \quad (A.1.3)$$

where the metric $g(\omega)$ is given by

$$g(\omega)_{nm} = \text{tr} \left[ \frac{\partial U(\omega)}{\partial \omega_n} U(\omega)^{-1} \left( \frac{\partial U(\omega)}{\partial \omega_m} U(\omega)^{-1} \right)^\dagger \right].$$

Instead of using the parameterization (A.1.3), it is sufficient to use the properties (A.1.1) and (A.1.2) for some group integrals. For $SU(3)$, a few examples are given below. The proofs can be found in chapter 3 of [8].

$$\begin{align*}
\int_{SU(3)} dU U_{ab} &= 0 \\
\int_{SU(3)} dU U_{ab} U_{cd} &= 0 \\
\int_{SU(3)} dU U_{ab} (U^\dagger)_{cd} &= \frac{1}{3} \delta_{ad} \delta_{bc} \\
\int_{SU(3)} dU U_{ab} U_{cd} U_{ef} &= \frac{1}{6} \epsilon_{ace} \epsilon_{bdf} \quad (A.1.4)
\end{align*}$$

For the calculation of the one-link integral in section 3.2, a generalization of (A.1.4) to arbitrary $N$ is needed. It was calculated in [15] and reads

$$\int_{SU(N)} dU \ U_{i_1 j_1} \cdots U_{i_N j_N} = \frac{1}{N!} \epsilon_{i_1 \cdots i_N} \epsilon_{j_1 \cdots j_N}. \quad (A.1.5)$$
A.2 Grassmann numbers

When fermions are included into the path integral formalism, their characteristic property, anti-symmetry under an exchange of quantum numbers, has to be assigned to the new field variables as well. To do so, fermionic fields are defined as Grassmann numbers. They obey the Grassmann property

\[ \eta_i \eta_j = -\eta_j \eta_i \quad \text{for} \quad 1 \leq i, j \leq N. \]  

(A.2.1)

By setting \( i = j \), this implies \( \eta_i^2 = 0 \) \( \forall i \). Therefore, every power series terminates after a finite number of terms \[8\]. The differentiation of Grassmann numbers is defined by the rules

\[ \frac{\partial}{\partial \eta_i} 1 = 0, \quad \frac{\partial}{\partial \eta_i} \eta_i = 1, \]  

(A.2.2)

\[ \frac{\partial}{\partial \eta_i} \frac{\partial}{\partial \eta_j} = -\frac{\partial}{\partial \eta_j} \frac{\partial}{\partial \eta_i}, \quad \frac{\partial}{\partial \eta_i} \eta_j = -\eta_j \frac{\partial}{\partial \eta_i} \quad \text{for} \ i \neq j. \]  

(A.2.3)

Given a polynomial

\[ A = a + \sum_i a_i \eta_i + \sum_{i<j} a_{ij} \eta_i \eta_j + \cdots + a_{12\ldots N} \eta_1 \cdots \eta_N, \quad a, a_i, \ldots, a_{12\ldots N} \in \mathbb{C}, \]

the integral \( \int d^N \eta \ A \in \mathbb{C} \) can be defined by the two requirements

\[ \int d^N \eta \ (\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 \int d^N \eta \ A_1 + \lambda_2 \int d^N \eta \ A_2, \]  

(A.2.4)

\[ \int d^N \eta \ \frac{\partial}{\partial \eta_i} A = 0. \]  

(A.2.5)

Together with the normalization

\[ \int d^N \eta \ \eta_1 \eta_2 \cdots \eta_N = 1, \]  

(A.2.6)

the integral yields (see \[8\])

\[ \int d^N \eta \ A = a_{12\ldots N}. \]  

(A.2.7)

The individual measures \( d\eta_i \) in the product measure

\[ d^N \eta = d\eta_N d\eta_{N-1} \cdots d\eta_1 \]

fulfill

\[ \int d\eta_i 1 = 0, \quad \int d\eta_i \eta_i = 1, \quad \int d\eta_i d\eta_j = -d\eta_j d\eta_i. \]
A Appendix

These relations are exactly the same as those for differentiation. Applying the linear transformation

\[ \eta_i' = \sum_{j=1}^{N} M_{ij} \eta_j, \quad M_{ij} \in \mathbb{C} \]

to (A.2.6) yields

\[
\int d^N \eta \eta_1 \eta_2 \cdots \eta_N = \int d^N \eta' \eta_1' \eta_2' \cdots \eta_N' \\
= \int d^N \eta' \sum_{i_1,i_2,\ldots,i_N} M_{1i_1}M_{2i_2} \cdots M_{Ni_N} \eta_{i_1} \eta_{i_2} \cdots \eta_{i_N} \\
= \int d^N \eta' \sum_{i_1,i_2,\ldots,i_N} M_{1i_1}M_{2i_2} \cdots M_{Ni_N} \epsilon_{i_1i_2\ldots i_N} \eta_{i_1} \eta_{i_2} \cdots \eta_{i_N} \\
= \det[M] \int d^N \eta' \eta_1 \eta_2 \cdots \eta_N.
\]

Hence the measure \(d^N \eta\) transforms under linear transformations via

\[ d^N \eta = \det[M] d^N \eta'. \quad \text{(A.2.8)} \]

A.3 Useful relations

Gaussian integral

We now want to calculate the Gaussian integral

\[
\int_{-\infty}^{\infty} dx \ e^{-ax^2+bx+c},
\]

since it appears in the calculation of the propagator in section 2.2. We start by completing the square

\[-ax^2 + bx = -a \left( x + \frac{b}{2a} \right)^2 - \left( \frac{b}{2a} \right)^2. \]

Next, we pull the factor \(e^{a\left(\frac{b}{2a}\right)^2+c}\) out of the integral and obtain

\[
\int_{-\infty}^{\infty} dx \ e^{-ax^2+bx+c} = e^{a\left(\frac{b}{2a}\right)^2+c} \int_{-\infty}^{\infty} dx \ e^{-a(x+\frac{b}{2a})^2}.
\]

By substituting \(y = \sqrt{a} \left( x + \frac{b}{2a} \right) \), we arrive at

\[
e^{a\left(\frac{b}{2a}\right)^2+c} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{a}} e^{-y^2} = \sqrt{\pi} e^{\frac{b^2}{4a} - c}, \quad \text{(A.3.1)}
\]

where we used the well-known identity

\[
\int_{-\infty}^{\infty} dx \ e^{-x^2} = \sqrt{\pi}.
\]
A.3 Useful relations

Multinomial theorem

When calculating the one-link integral, we encounter expressions like $(\bar{\chi}(y)U\chi(x))^k$. To see how the Grassmann property affects such expressions, it is useful to write down the sum over color-components explicitly and to apply the \textit{multinomial theorem} to it. The theorem reads

\[ (x_1 + x_2 + \cdots + x_n)^k = \sum_{k_1 + \cdots + k_n = k} \binom{k}{k_1, \ldots, k_n} x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n}. \tag{A.3.2} \]

Grassmann integral identity

We want to prove the identity

\[ I = \int d\chi(x) d\bar{\chi}(x) \int dU \ e^{\bar{\chi}(x)\chi(x)+\bar{\chi}(x)U\chi(y)-\bar{\chi}(y)U^\dagger\chi(x)} = e^{\bar{\chi}(y)\chi(y)}, \tag{A.3.3} \]

which is used to determine coefficients for the one-link integral. Therefore, we perform the transformation

\[ \chi'(x) = U^\dagger \chi(x) \]
\[ \bar{\chi}'(x) = \bar{\chi}(x)U. \]

The measures $d\chi(x)$ and $d\bar{\chi}(x)$ transform according to (A.2.8), introducing the factors $\text{det}[U]$ and $\text{det}[U^\dagger]$. Since $U^\dagger U = 1$ and $\text{det}[U]\text{det}[U^\dagger] = 1$, the integral simplifies to

\[ I = \int d\chi'(x) d\bar{\chi}'(x) \int dU \ e^{\bar{\chi}'(x)\chi'(x)+\bar{\chi}'(x)\chi(y)-\bar{\chi}(y)\chi'(x)} \]
\[ = \int d\chi'(x) d\bar{\chi}'(x) \int dU \ e^{(\bar{\chi}'(x)-\bar{\chi}(y))(\chi'(x)+\chi(y))} + \bar{\chi}(y)\chi(y) \]
\[ = e^{\bar{\chi}(y)\chi(y)} \int d\chi''(x) d\bar{\chi}''(x) \int dU \ e^{\bar{\chi}''(x)\chi''(x)}. \]

In the last step, we defined new integration variables

\[ \chi''(x) = \chi'(x) - \chi(y) \]
\[ \bar{\chi}''(x) = \bar{\chi}'(x) - \bar{\chi}(y). \]

By using (A.1.1) and the Matthews-Salam formula (see chapter 5 of [8]), we arrive at

\[ I = e^{\bar{\chi}(y)\chi(y)}. \]
\begin{thebibliography}{15}


\end{thebibliography}
Eigenständigkeitserklärung


Bielefeld, den 26. September 2016

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Unterschrift