Eva Grünwald

Comparison of Taylor- and Fugacity-Expansion in the Effective Center Model

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Betreuer: Univ.-Prof. Dr.rer.nat. Christof Gattringer
Institut für Physik

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Abstract

The exploration of the phase diagram of quantum chromodynamics (QCD) is one of the most challenging and yet essential quests of theoretical particle physics nowadays. Not only does the QCD phase diagram provide insight into processes in neutron stars, it is also crucial to gather information about the very first moments of the universe. At present day, there are running experiments investigating the transition to an extreme phase of matter, the so-called quark-gluon plasma, which still lacks a proper theoretical description.

In this work, we compare two main expansion techniques used in QCD at finite density, Taylor- and fugacity expansion, and study their capability of exploring the phase diagram of the effective center model, a QCD related model. To this purpose, we calculate observables in the critical temperature region and use results obtained in terms of a flux representation as reference data to test the reliability and the limitations of Taylor- and fugacity series expansion. We show that the fugacity expansion converges until the complex action problem becomes severe, whereas the Taylor expansion is reliable only in a very small range of chemical potential in the model under consideration. Both expansion techniques are not able to completely reproduce the phase diagram of the effective center model. The assessment of the quality of the perturbative approaches can be used to improve these techniques for their application in QCD.
To my family.

"The family is one of nature's masterpieces."
George Santayana
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1. Introduction

The Standard Model of particle physics is the accepted theory of the elementary constituents of matter in the universe and the fields via these interact \[1,2\]. In this theory, the elementary particles are fermions and the particles associated with the interaction fields are bosons \[3,4\]. The Standard Model treats three out of the four fundamental forces in terms of so called gauge theories. One of the fundamental forces considered in the Standard Model is the strong interaction between quarks mediated by gluons which gives rise to the formation of hadrons, for example the proton. To understand the strong force in detail, a mathematical description was searched for and it is generally accepted, that quantum chromodynamics (QCD) is the mathematical framework of the strong interaction.

QCD is a gauge theory based on the SU(3) colour group, a non-Abelian group. The non-commutativity of the gauge group is connected to a property of QCD called asymptotic freedom and to quark confinement. Asymptotic freedom means that forces between two close-by quarks become small which allows for perturbative calculations of processes at high energies. However, quark confinement which manifests at large separations of two quark sources can only be treated non perturbatively \[5\].

A powerful non-perturbative approach to the theory of quarks and gluons is the lattice formulation of QCD (LQCD) by Wilson \[6\], which made it possible to access a wide range of phenomenological questions at low energies.

Altough LQCD is a well established research tool nowadays and achieved a lot of successes in recent years, there are still questions to be answered. For example the finite temperature and finite density behaviour of QCD is one of the major fields of interest in theoretical particle physics today.

The reason for the difficulties in the determination of the phase diagram of QCD in terms of lattice simulations is the so-called complex action problem which manifests itself at finite chemical potential, hindering the standard method of LQCD, the Monte Carlo approach. There have been several attempts to bypass the complex action problem.

In this work, two methods to overcome the complex action problem are of main interest. Namely rewriting lattice field theories with the help of new variables and series expansion methods.
Rewriting techniques bypass the complex action problem by finding an exact transformation to a representation where the partition function has only real and positive parts, allowing for Monte Carlo techniques. This representation is called flux representation. One theory for which the action could be rewritten in this manner and a phase diagram could be shown is the effective center model, a $\mathbb{Z}_3$ spin model [7]. The phase diagram (Figure 1.1) shows the qualitative behaviour and the mass dependence as expected for full QCD. There is no critical end point when only center degrees of freedom are considered [7].

In this research we use the outcome of the flux representation to test the reliability and the limitations of the two main expansion techniques used in QCD, Taylor- and fugacity expansion, in the effective center model.

For this purpose we are going to review basic lattice gauge field theory in the rest of this chapter, before investigating the fugacity series in Chapter 2 and two Taylor expansion methods in Chapter 4. Chapter 3 shortly treats the complex action problem in the effective $\mathbb{Z}_3$ spin model. In Chapter 5 we compare the expansion technique results to the outcome of the flux representation, testing the reliability and the breakdown of the expansion technique methods.
The following sections give short introductions to gauge fields and phase transitions on the lattice, and to Monte Carlo simulations. However, the sophisticated and wide ranging research field of LQCD can not be treated thoroughly in this thesis. There are some excellent books on the topic, for example [8], [5], [9], [10].
1. Introduction

1.1. Lattice Formulation of Gauge Field Theories

The basic formulation of a theory can be given in terms of its Lagrangian density. The Lagrangian density of free fermions in QCD can be obtained from the Dirac equation formulated in Minkowski space. In Lattice QCD one works in the Euclidean space. The transformation from the Minkowski space to the Euclidean space is called Wick rotation. The Wick rotation makes methods of statistical mechanics in quantum field theory applicable, due to structural similarities of the partition function.

We begin our way towards QCD on the lattice with the introduction of gauge theories. After that, we write down the Wick rotated "free fermion action" in the Euclidean continuum space. As we will see, this action is not gauge invariant a priori. The enforcement of the gauge principle for this action will lead to the introduction of so called gauge fields. Taking into account also the gluonic part of the action, we will be able to write down the Euclidean continuum action. This action has to be quantized in order to get from the classical to the field theoretical picture. However, the quantized theory then suffers from infinite contributions, making the calculation of observables impossible. Only a regularized theory can give physical observables. A prominent way of regularization is the formulation of the theory on a discrete space-time lattice, LQCD.

In this section, we give some details of the way from the continuum to the lattice formulation of QCD, following [8] mostly. The discretized theory is then ready to calculate observables in Monte Carlo simulations.

We already mentioned, that the purpose of this thesis is the analysis of the confinement-deconfinement transition in a QCD related model at finite density (with the purpose to compare the outcome to already existing results from flux representation methods). For full QCD, this analysis is very challenging. However, when we concentrate on pure gluodynamics, there is a well defined order parameter, namely the Polyakov loop. For this reason, we take only the gluonic degrees of freedom into account when it comes to calculating observables on the lattice.

Let us start with the introduction of the important concept of gauge theories.

1.1.1. SU(N) Gauge Theories

The essence of the Standard Model are Yang-Mills theories. These theories describe the behavior of elementary particles using the non-Abelian Lie groups $SU(N)$.

The Necessity of Gauge Fields

The key feature of Yang-Mills theories is their invariance under a certain group of local transformations which are called gauge transformations. This requirement is called the
gauge principle. The idea of Yang and Mills was most certainly inspired by the well understood theory of quantum electrodynamics (QED) with its Abelian $U(1)$ symmetry group. In QED, the introduction of a covariant derivative recovers the gauge invariance of the theory. In the following, it will be shown that a similar treatment ensures the gauge invariance of Yang-Mills theories.

Since the gauge principle demands that the Lagrangian of the theory must be invariant under local gauge transformations, we introduce the action of a free fermion in order to analyze if it is a priori invariant under gauge transformations (and treat the bosonic part later).

The free fermion action in Euclidean space reads

$$S^0_F[\psi, \bar{\psi}] = \sum_{f=1}^{N_f} \int \bar{\psi}^{(f)}(x) \left( \gamma_\mu \partial_\mu + m^{(f)} \right) \psi^{(f)}(x) d^4 x,$$  \hspace{1cm} (1.1)

where $\gamma^\mu$ are the Euclidean Dirac matrices, which fulfil $\{\gamma_\mu, \gamma_\nu\} = 2 \delta_{\mu, \nu} \mathbb{1}$. The fields representing the quarks in the theory are given by the Dirac-4-Spinor

$$\psi(x) = \psi(x)^f_{\alpha,c}$$  \hspace{1cm} (1.2)

and the corresponding antiparticles are represented by

$$\bar{\psi}(x) = \bar{\psi}(x)^f_{\alpha,c}.$$  \hspace{1cm} (1.3)

where all indices defining the particle are shown explicitly. The flavor index is $f = 1, 2, 3, ..., N_f$ and $x = (x_1, x_2, x_3, x_4)$ denotes the space-time position and $\alpha = 1, 2, 3, 4$ denotes the Dirac indices. For reasons of clarity, these indices are omitted in the following.

Now, we need to specify the gauge transformations. The fields representing the quarks and antiquarks in our theory transform under some representation $\Omega(x) \in SU(N)$ as

$$\psi(x) \rightarrow \psi(x)' = \Omega(x) \psi(x),$$  \hspace{1cm} (1.4)

$$\bar{\psi}(x) \rightarrow \bar{\psi}(x)' = \bar{\psi}(x) \Omega(x)^\dagger.$$  \hspace{1cm} (1.5)

The transformation matrices have determinant one, are unitary and can be parametrized as

$$\Omega(x) = e^{-i \Theta^a(x) \tau^a},$$  \hspace{1cm} (1.6)

where $\Theta^a(x)$ denote some space dependent parameters. It is very important to notice, that with $\Omega(x)$ applied to the fermion fields, we perform a local transformation. It is different for every space-time position $x$. Furthermore, $\tau^a$ are the generators of the
Lie Algebra. For $SU(N)$, these are $N^2 - 1$ generators and they fulfil the commutation relation
\[
[\tau^a, \tau^b] = if^{abc}\tau^c,
\] (1.7)
where $f^{abc}$ are the structure constants of the group. In contrast, the rhs. of relation (1.7) is zero for Abelian groups by definition.

If we apply the gauge transformations (1.4), (1.5) to the action (1.1), we see that the mass term obeys the gauge principle, it is invariant. However, the derivative term is not. The introduction of a ”covariant derivative” can maintain the gauge invariance of (1.1). It is given by
\[
D_\mu = \partial_\mu + igA_\mu(x),
\] (1.8)
where a new constant $g$ and new fields $A(x)$, gauge fields, are introduced. These additional fields are required by the gauge principle. The gauge fields are elements of the Lie algebra $su(N)$ and related to the generators $\tau$ of the gauge group $SU(N)$ via
\[
A_\mu = A^a_\mu(x)\tau^a.
\] (1.9)
The transformation of the gauge fields is given by
\[
A_\mu(x) \rightarrow A'_\mu(x) = \Omega(x)A_\mu(x)\Omega^\dagger(x) + i(\partial_\mu\Omega(x))\Omega^\dagger(x),
\] (1.10)
and the transformation of the covariant derivative reads
\[
D_\mu(x) \rightarrow D'_\mu(x) = \Omega(x)D_\mu(x)\Omega^\dagger(x).
\] (1.11)

It can be shown, that the introduction of the covariant derivative (implying the introduction of gauge fields) and the transformation properties (1.10), (1.11) ensure the gauge invariance of the fermionic part of the QCD action \[8\], which then reads
\[
S_F[\psi, \bar{\psi}, A] = \sum_{f=1}^{N_f} \int \bar{\psi}^{(f)}(x) \left( \gamma_\mu \partial_\mu + igA_\mu(x) + m^{(f)} \right) \psi^{(f)}(x)d^4x.
\] (1.12)

We stated that the Lagrangian density should be invariant under gauge transformations. The action is connected to the Lagrangian density in the following way
\[
S_E = S_F + S_G = \int \mathcal{L}_E d^4x.
\] (1.13)
So far, we only treated the fermionic part of the action, $S_F$. In the following, we are going to investigate the gluonic part of the action ($S_G$) which is sometimes called the Yang-Mills term.
1.1. Lattice Formulation of Gauge Field Theories

The Yang Mills Term in the Euclidean Continuum Action

In order to construct the bosonic part of the continuum action, it is possible to write down a functional of the gauge fields $A_\mu$, the field strength tensor:

$$F_{\mu\nu}(x) = -\frac{1}{g} [D_\mu(x), D_\nu(x)] = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) + ig [A_\mu(x), A_\nu(x)].$$  \hspace{1cm} (1.14)

It can be further verified, that a valid expression for the invariant continuum gauge action is then given by

$$S_G[A] = \frac{1}{2g^2} \int tr[F_{\mu\nu}(x)F_{\mu\nu}(x)]d^4x.$$  \hspace{1cm} (1.15)

A thorough analysis of the derivation of the continuum Euclidean action is given in [8], but this very short and basic summary suffices to bring some important facts of the theory to attention. Firstly, we saw that the gauge principle demands the introduction of gauge fields and secondly, the non-vanishing commutator in (1.14) gives rise to the self-interaction of gluons. Furthermore, we can identify the constant introduced in (1.8) with the bare coupling strength of the theory.

So far, we showed the Euclidean action of a continuum gauge field theory which is a classical theory. The path integral approach can be used to quantize the theory in order to obtain a quantum gauge field theory. In the following, we are going to sketch the idea of path integration.

The Path Integral

The path integral approach relies on the idea of taking into account all possible trajectories of a given field instead of concentrating on one distinct time evolution. To this purpose, an infinite dimensional functional integral is introduced. It is then possible to relate the partition function $Z$ of the quantized Euclidean gauge field theory to an integration over all possible field configurations in the following way

$$Z = \int \mathcal{D}[\psi] e^{-S_E[\psi]}.$$  \hspace{1cm} (1.16)

The integration measure $\mathcal{D}[\psi]$ denotes the integration measure over all field configurations $\psi$ and will be given a mathematically rigorous definition below, when we introduce the lattice.

In this manner, a quantized expression for the partition function can be found by using the classical continuum action (1.12),(1.15). Moreover, all thermodynamic quantities can be obtained from (1.16), at least in principle. The practical difficulties lie in the determination of the integration measure and even worse, (1.16) can not yield physical results, meaning finite results, since it includes diverging contributions. To solve the
1. Introduction

problem of the diverging contributions, different regularization techniques are applied.

A very important method is the lattice regularization, on which the focus of our work lies. But how can one put a gauge field theory on a space-time lattice? The answer to this will be sketched in what follows.

1.1.2. The Lattice Formulation of a Gauge Field Theory

Firstly, we introduce our finite space-time lattice as

$$\Lambda = \{ n = (n_1, n_2, n_3, n_4) | n_1, n_2, n_3 = 1, 2, ..., N_s \land n_4 = 1, 2, ..., N_t \}.$$  \hfill (1.17)

Additionally, we call the lattice spacing $a$, implying the same spatial and temporal separation of lattice sites. We can now think of the fermion fields sitting on the points $x = n \cdot a$ of the space-time lattice $\Lambda$. Secondly, we separate the fermionic part of the action $S_F$ once more from the bosonic part $S_G$ in order to put fermions and bosons successively on the lattice.

Naive Fermions on the Lattice

As already mentioned, the fermion fields sit on the lattice points $n \in \Lambda$, therefore, we introduce the lattice fermion fields $\Psi(n)$:

$$\psi(x) \rightarrow \Psi(n),$$  \hfill (1.18)

and

$$\bar{\psi}(x) \rightarrow \bar{\Psi}(n).$$  \hfill (1.19)

For reasons of simplicity, we start by putting the non-gauge invariant Euclidean free fermion action $S^0_F$ \hfill (1.1) on the lattice. Since we already put the fermion fields $\psi$ and $\bar{\psi}$ on the lattice, the only part left to discretise is the derivative $\partial_\mu$. It can be replaced by the central difference quotient

$$\partial_\mu \psi(x) \rightarrow \frac{\Psi(n + \hat{\mu}) - \Psi(n - \hat{\mu})}{2a} + O(a)$$  \hfill (1.20)

where $\hat{\mu}$ is the unit vector in $\mu$-direction. This gives the free fermion action on the lattice

$$S^0_F[\Psi, \bar{\Psi}]_{LAT} = a^4 \sum_{n \in \Lambda} \bar{\Psi}(n) \left( \sum_{\mu=1}^{4} \gamma_\mu \frac{\Psi(n + \hat{\mu}) - \Psi(n - \hat{\mu})}{2a} + m \Psi(n) \right),$$  \hfill (1.21)

where the discretization made a sum over all lattice points out of the integral.

The attentive reader will have noticed that the crucial gauge principle is not yet considered in \hfill (1.21). The demand for the invariance of the action under the gauge transformation lead to the need for gauge fields in the continuum theory. A similar requirement for additional fields is to be expected for the lattice formulation of the gauge theory. These gauge fields can be interpreted quite pictorially on the lattice.
1.1. Lattice Formulation of Gauge Field Theories

**Link Variables**

We define the gauge transformation for the fermion fields on the lattice under an element of the group $SU(N)$ denoted by $\Omega(n)$ to be

$$\Psi(n) \to \Psi'(n) = \Omega(n)\Psi(n)$$  \hspace{1cm} (1.22)

and

$$\bar{\Psi}(n) \to \bar{\Psi}'(n) = \bar{\Psi}(n)\Omega(n)\dagger.$$  \hspace{1cm} (1.23)

The next step is to apply the gauge transformations to the action (1.21). We find that the mass term is again trivially invariant under the local gauge transformation, but the derivative term is not. For example

$$\bar{\Psi}(n)\Psi(n + \hat{\mu}) \to \bar{\Psi}'(n)\Psi'(n + \hat{\mu}) = \bar{\Psi}(n)\Omega(n)\dagger\Omega(n + \hat{\mu})\Psi(n + \hat{\mu})$$  \hspace{1cm} (1.24)

In order to maintain gauge invariance, we introduce new field variables, as we did in the continuum. Let us call them $U_\mu(n)$, which shall be elements of $SU(N)$. We gauge transform again and get

$$\bar{\Psi}'U'_\mu(n)\Psi'(n + \hat{\mu}) = \bar{\Psi}(n)\Omega(n)\dagger U'_\mu(n)\Omega(n + \hat{\mu})\Psi(n + \hat{\mu}).$$  \hspace{1cm} (1.25)

It is obvious that if $U_\mu(n)$ transforms as

$$U_\mu(n) \to U'_\mu(n) = \Omega(n)U_\mu(n)\Omega(n + \hat{\mu})\dagger,$$  \hspace{1cm} (1.26)

the additional terms which ruin the gauge invariance of (1.21) cancel since the transformation matrices $\Omega(n)$ are unitary.

We mentioned a pictorial interpretation of the gauge fields. The $SU(N)$ elements $U_\mu(n)$ connect the site $n$ and the site $n + \hat{\mu}$ on the lattice, they are sitting on the links between the lattice sites. This interpretation would imply that you could also reverse this connection. This is indeed possible if we define

$$U_{-\mu}(n) = U_\mu(n - \hat{\mu})\dagger.$$  \hspace{1cm} (1.27)

The reversed link variables transform as follows

$$U_{-\mu}(n) \to U'_{-\mu}(n) = \Omega(n)U_{-\mu}(n)\Omega(n - \hat{\mu})\dagger.$$  \hspace{1cm} (1.28)

Having taken into account the gauge principle, we can write down the discretized version of (1.12), the so-called naive fermion action, which reads

$$S_F[\Psi, \bar{\Psi}, U]_{\text{LAT}} = a^4 \sum_{n \in \Lambda} \bar{\Psi}(n) \left( \sum_{\mu=1}^{4} \gamma^\mu U_\mu(n)\Psi(n + \hat{\mu}) - U_{-\mu}(n)\Psi(n - \hat{\mu}) \right) + m\Psi(n).$$  \hspace{1cm} (1.29)

The adjective "naive" refers to the problem of fermion doubling from which (1.29) suffers. The doubling problem can also be solved by the introduction of additional terms, we refer to [8] for details again.
1. Introduction

Figure 1.2.: Graphical interpretation of the gauge fields $U_\mu(n)$ and $U_\mu(n - \hat{\mu})^\dagger$ as link variables (from [8]).

**Gauge Fields on the Lattice**

We introduced the gluon fields on the lattice as link variables and are now concerned with their gauge invariant action. This means we are looking for gauge invariant objects built out of the links $U_\mu$. Let $\mathcal{P}$ be a path of $k$ links, connecting the two lattice sites $n_0$ and $n_1$

$$P[U] = U_{\mu_0}(n_0) U_{\mu_0}(n_0 + \hat{\mu}_0) ... U_{\mu_k-1}(n_1 - \hat{\mu}_{k-1}) \equiv \prod_{(n,\mu) \in \mathcal{P}} U_\mu(n). \quad (1.30)$$

From the transformation properties of the link variables (1.26) and (1.28) it follows, that only the two endpoints of the path $n_0$ and $n_1$ contribute under the gauge transformation

$$P[U] \rightarrow P[U'] = \Omega(n_0) P[U] \Omega(n_1)^\dagger. \quad (1.31)$$

Our path $\mathcal{P}$ (1.30) is therefore not gauge invariant. An obvious way out seems to be $n_0 = n_1 = n$, which means closing the path $\mathcal{P}$ to a loop $\mathcal{L}$, such that

$$L[U'] = \Omega(n) P_c[U] \Omega(n)^\dagger, \quad (1.32)$$

where the index $c$ stresses that the path is closed. But now we have to find a way in which we are allowed to interchange $\Omega$ and $P$ to obtain gauge invariance. Taking the trace does the trick. The property of cyclic permutation allows to exploit the unitary of $\Omega(n)$:

$$L[U'] = \text{tr} \left[ \Omega(n_0) \prod_{(n,\mu) \in \mathcal{L}} U_\mu(n) \Omega(n_0) \right] = \text{tr} \left[ \prod_{(n,\mu) \in \mathcal{L}} U_\mu(n) \right] = L[U]. \quad (1.33)$$

The trace over a closed path of link variables, a loop $\mathcal{L}$, is a gauge invariant object. Such loops are not only essential for the construction of the gluonic part of the action, they can also be used as physical observables.

For now, we are interested in finding a gauge invariant gluonic action. The shortest closed loop on a lattice is the so-called plaquette.

$$U_{\mu\nu}(n) = U_\mu(n) U_\nu(n + \hat{\mu}) U_{-\mu}(n + \hat{\mu} + \hat{\nu}) U_{-\nu}(n + \hat{\nu}) = U_\mu(n) U_\nu(n + \hat{\mu}) U_\mu(n + \hat{\nu}) U_\nu(n)^\dagger. \quad (1.34)$$
1.1. Lattice Formulation of Gauge Field Theories

The first one to use the plaquette (Figure 1.3) in order to construct a gauge invariant action for SU(3) was K. Wilson. It reads

\[ S_G[U] = 2 g^2 \sum_{\mathbf{n} \in \Lambda} \sum_{\mu < \nu} \text{Re} \, \text{tr} \left[ 1 - U_{\mu\nu}(n) \right], \quad (1.35) \]

and is called Wilson gauge action. It approximates the continuum action up to order \( O(a)^2 \) and for \( a \to 0 \), the naive continuum limit is recovered.

The True Continuum Limit

In order to calculate observables, we introduced a cut-off with the discretization of the theory. As a consequence, all quantities calculated on the lattice depend on the lattice spacing \( a \). Especially, the bare coupling constant \( g \) depends on \( a \) (running coupling constant). The behaviour of the running coupling constant is described by the \( \beta \)-function

\[ \beta(g(a)) = -\frac{\partial g(a)}{\partial \ln a}. \quad (1.36) \]

In the naive continuum limit \( a \to 0 \), this dependency of the coupling on the lattice spacing is not considered. However, it can be shown, that \( \beta \propto \frac{1}{a} \), this means for

\[ \beta \to \infty \Rightarrow a \to 0 \quad (1.37) \]

and we may construct a continuum limit by considering \( \beta \to \infty \). But since \( V_{\text{LAT}} \propto a^4 \), also the lattice shrinks. Increasing the spatial lattice extent

\[ N_s \to \infty, \quad (1.38) \]
1. Introduction

and simultaneously the temporal extent

\[ N_t \to \infty, \quad \text{(1.39)} \]

prevents the lattice from vanishing and is called the thermodynamic limit.

1.1.3. Observables on the Lattice

So far, we put the fermionic part and the gluonic part of the Euclidean continuum action on a space time lattice. This was done because without a regularization the theory suffered from infinite contributions, making the calculation of observables impossible.

As already mentioned, we are going to use the Polyakov loop as order parameter for confinement (which is only possible in a pure gauge theory) and discard the fermionic part of the theory when it comes to calculating observables. The expectation value of an arbitrary operator \( \hat{O} \) in terms of the gluonic degrees of freedom on the lattice then reads

\[
\langle \hat{O} \rangle = \frac{1}{Z_G} \int \mathcal{D}[U] e^{-S_G[U]} O[U], \quad \text{(1.40)}
\]

where \( S_G \) is the gluonic part of the action on the lattice and \( Z_G = Z_G^{\text{LAT}} \) denotes the gluonic partition function on the lattice.

The measure over all gauge configurations can now be mathematically rigorously defined as the product measure over all link variables,

\[
\int \mathcal{D}[U] = \prod_{n \in \Lambda} \prod_{\mu=1}^{4} \int dU_{\mu}(n), \quad \text{(1.41)}
\]

where \( U_{\mu}(n) \in SU(3) \) and the integration \( dU_{\mu}(n) \) is therefore over the whole group manifold of \( SU(3) \). A suitable measure for the integration over a continuous compact group which also leaves \( Z_G \) invariant under gauge transformations is the Haar measure. For details on the Haar measure, we refer again to [8].

As long as the gauge is not fixed, the observables have to be gauge invariant as well, because otherwise their expectation value would vanish. A functional \( O[U] \) of the links \( U \) which qualifies as an observable therefore must obey

\[
O[U] = O[\Omega U \Omega^\dagger] = O[U'], \quad \text{(1.42)}
\]

i.e., must be gauge invariant.
1.1. Lattice Formulation of Gauge Field Theories

Introduction of the Wilson Loop

We have already shown (1.33) that a traced loop of link variables

\[ L[U] = \text{tr} \left[ \prod_{(n,\mu) \in \mathcal{L}} U_{\mu}(n) \right] \]  

(1.43)

is a gauge invariant object and a candidate for an observable in this way. One possibility of such a closed loop is shown in Figure 1.4.

Figure 1.4.: Sketch of a closed loop out of temporal and spatial transporters (1.46).

The trace of this loop is called Wilson loop.

The Wilson loop is the trace of the product of links in temporal and in spatial direction, where the temporal transporters are

\[ T(n, n_t) = \prod_{t=1}^{n_t-1} U_4(n, t), \]  

(1.44)

and the spatial transporters - which connect two spatial points - are defined as

\[ S(m, n, n_t) = \prod_{(k,j) \in \mathcal{C}_{m,n}} U_j(k, n_t). \]  

(1.45)

In this manner, spatial transporters allow to move in the spatial direction on the lattice, whereas the time transporters allow to propagate in time on the lattice.

The loop \( \mathcal{L} \) out of temporal transporters and spatial Wilson lines depicted in Figure 1.4 then reads

\[ \mathcal{L} = (m, n_t) \overset{S}{\rightarrow} (n, n_t) \overset{T_t}{\rightarrow} (n, 0) \overset{S_t}{\rightarrow} (m, 0) \overset{T}{\rightarrow} (m, n_t). \]  

(1.46)
1. Introduction

The Wilson loop $W_L$ is obtained by taking the trace, because of the required gauge invariance of observables

$$W_L = \text{tr} \left[ S(m, n, n_t) T(n, n_t) S(m, n, 0) \right] = \text{tr} \left[ \prod_{(k, \mu) \in L} U_\mu(k) \right]. \quad (1.47)$$

The expectation value of (1.47) is related to the potential $V(a| m - n|)$ between a static quark-antiquark pair, where the quark is sitting at lattice point $n$ and the antiquark at the site $m$ (or vice versa) via

$$\langle W_L \rangle \propto \exp \left\{ -n_t a V(r) \right\} \left( 1 + O(e^{-n_t a \Delta E}) \right), \quad (1.48)$$

where $r = a| m - n|$ and $n_t$ is the time extent of $W_L$. The energy difference between $V(r)$ and the first excited quark-antiquark pair state is denoted by $\Delta E$.

Relation (1.48) can be understood in terms of Euclidean correlators. For that reason, we are now going on a short side trip, having a glimpse at Euclidean correlators.

The Euclidean Correlator

A very important quantity, which is here only mentioned shortly, is the Euclidean correlator between two arbitrary operators $\hat{O}_1$ and $\hat{O}_2$ which reads

$$\lim_{T \to \infty} \frac{1}{Z_T} \text{tr} \left[ e^{-\left( T-t \right) \hat{H}} \hat{O}_2 e^{-\hat{H}T} \hat{O}_1 \right] = \sum_n \langle 0| \hat{O}_2 | n \rangle \langle n| \hat{O}_1 | 0 \rangle e^{-tE_n}, \quad (1.49)$$

where we have abandoned the lattice formulation for a moment. $Z_T = \text{tr} \left[ e^{-T\hat{H}} \right]$ is called partition function, where $\hat{H}$ is the Hamiltonian of the system and $T, t$ are real valued and non negative. The right hand side of (1.49) is obtained by inserting eigenstates of $\hat{H}$. The sum runs over all physical states $| n \rangle$. Furthermore, the right hand side contains matrix elements which are weighted according to the energy eigenvalues of the system, denoted by $E_n$. The weight factor is time dependent as well. From (1.49), the energies $E_n$ can be extracted.

The Euclidean correlator can also be expressed in terms of the path integral formalism

$$\lim_{T \to \infty} \frac{1}{Z_T} \text{tr} \left[ e^{-\left( T-t \right) \hat{H}} \hat{O}_2 e^{\hat{H}T} \hat{O}_1 \right] = \frac{1}{Z_T} \int D[\Psi] e^{-\mathcal{S}_E[\Psi]} \langle O_2(\cdot, t)| O_1(\cdot, 0) \rangle. \quad (1.50)$$

The integral sums now over all possible field configurations. The path integral in this way allows for the expression of operator valued functions (l.h.s.) in terms of functionals (r.h.s.) weighted with the so-called Boltzmann factor containing the classical Euclidean action $\mathcal{S}_E[\Psi]$. 

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The Euclidean correlator between two operators on the lattice \( \hat{O}_1[U] \) and \( \hat{O}_2[U] \) can be given in terms of the path integral as well and reads
\[
\langle \hat{O}_2(t)\hat{O}_1(0) \rangle = \frac{1}{Z_{LAT} G} \int D[U] e^{-S^{LAT}_{G}[U]}O_1[U]O_2[U],
\]
where the operators on the r.h.s. are now functionals and the exponent contains the gluonic part of the Euclidean action on the lattice. The important point is here, that the r.h.s. can be evaluated numerically using methods from statistical mechanics.

**Physical Interpretation of the Wilson Loop**

With the definition of the Euclidean correlator at hand, we are now going to have a closer look at the physical meaning of the Wilson loop
\[
W_L = \text{tr} \left[ S(m,n,t)S(m,n,0)T(n,t) \right] = \text{tr} \left[ \prod_{(k,\mu) \in \mathcal{L}} U_{\mu}(k) \right].
\]
To this purpose, we work in the so-called temporal gauge, meaning
\[
T(m,n_t) = 1
\]
where we set all temporal links to 1. The expectation value of the Wilson loop then reads
\[
\langle W_L[U] \rangle = \langle \text{tr} S(m,n,t)S(m,n,0)T(n,t) \rangle = \sum_k \langle 0|\hat{S}(m,n)|k \rangle \langle k|\hat{S}(m,n)|0 \rangle e^{-tE_k},
\]
where \( E_1 \) can be identified with \( V(r) \), the potential of a static quark antiquark pair and \( t = an_t \), see (1.48).

**The Polyakov Loop and Confinement**

An important modification of the Wilson loop on the lattice is the Polyakov loop. It is a product of all time-like links at a certain spatial point \( m \) (thermal Wilson line). If we gauge the spatial Wilson lines to 1, we get two disconnected temporal lines which wind around the lattice in time direction - due to the periodic boundary conditions - and are closed loops in this manner. If we take the trace of this quantity, we get a well
defined gauge invariant observable on the lattice.

The local Polyakov loop at spatial site \( \mathbf{m} \) is defined as
\[
P(\mathbf{m}) = \text{tr} \left[ N_t - 1 \prod_{j=0}^{N_t-1} U_4(\mathbf{m}, j) \right].
\] (1.57)

For \( n_T \to N_T \), the expectation value of the Wilson loop (1.56) in temporal gauge becomes the Euclidean correlator of two Polyakov loops at spatial points \( \mathbf{m} \) and \( \mathbf{n} \). It reads
\[
\langle \overline{P(\mathbf{m})} P(\mathbf{n}) \rangle \propto e^{-N_T a V(r)} (1 + \mathcal{O}(e^{-N_T a \Delta E}))
\] (1.58)
and is in this way related to the potential between a pair of infinitely heavy quark and antiquark, separated by the distance \( r = a|n - m| \). We have not discussed \( V(r) \) so far.

The potential between a static quark-antiquark pair may be parameterized
\[
V(r) = A + \frac{B}{r} + \sigma r.
\] (1.59)

\( A \) is an additive constant, \( B \) is the constant giving the strength of the Coulomb term and \( \sigma \) is called the string tension and is also a constant. Because for \( r \to \infty \), only a vanishing \( \sigma \) allows for a constant amount of energy to separate the quark-antiquark pair, \( \sigma r \) is called the confinement part.

\[
\lim_{r \to \infty} V(r) = \infty, \quad \text{if} \quad \sigma \neq 0 \quad \rightarrow \text{confined}.
\] (1.60)

\[
\lim_{r \to \infty} V(r) = \text{const.}, \quad \text{if} \quad \sigma = 0 \quad \rightarrow \text{deconfined}.
\] (1.61)

For large distances \( r \to \infty \), the correlator (1.58) connected to the static quark potential gives
\[
\lim_{r \to \infty} \langle \overline{P(\mathbf{m})} P(\mathbf{n}) \rangle = \langle \overline{P(\mathbf{m})} \rangle \langle P(\mathbf{n}) \rangle.
\] (1.62)

Because of the invariance under translation of the spatial points on the lattice, this can be written as
\[
\lim_{r \to \infty} \langle \overline{P(\mathbf{m})} P(\mathbf{n}) \rangle = |\langle P \rangle|^2
\] (1.63)
and therefore
\[
|\langle P \rangle|^2 \propto e^{-N_T a V(\infty)},
\] (1.64)
which relates the expectation value of the Polyakov loop to the potential \( V(r) \) at \( r = \infty \).

In the confined phase,
\[
\lim_{r \to \infty} V(r) \to \infty \Rightarrow e^{-N_T a V(r)} \to 0 \Rightarrow |\langle P \rangle|^2 \to 0.
\] (1.65)
A finite value for the Polyakov loop means therefore a finite potential \( V(r) \) between quark and antiquark, the system is in the deconfined phase.

The expectation value of a single Polyakov loop can also be interpreted as

\[
|\langle P \rangle| \propto e^{-tF_q}, \quad (1.66)
\]

where \( F_q \) denotes the free energy of a single colour charge.

Summarizing,

\[
\langle P \rangle = 0 \rightarrow \text{confined phase},
\]

\[
\langle P \rangle \neq 0 \rightarrow \text{deconfined phase}. \quad (1.67)
\]

**Analogy to Statistical Mechanics**

At the very beginning of this chapter, we mentioned the Wick rotation as transformation from the Minkowski space to the Euclidean space \((x_0 \to i x_4)\). We also mentioned, that it is used to reveal the analogies of quantum field theory and statistical mechanics. With the definition of the path integral, we can illustrate this similarity now in terms of the partition functions

\[
Z_{QCD} = \int \mathcal{D}[\Psi] e^{iS_{QCD}} \rightarrow Z_{LAT} = \int \mathcal{D}[\Psi] e^{-S_{QCD}}, \quad (1.68)
\]

therefore

\[
Z_{LAT} = \int \mathcal{D}[\Psi] e^{-S_{QCD}} \leftrightarrow Z_{STAT} = \sum_s e^{-\beta H[s]}, \quad (1.69)
\]

\( H \) is the Hamiltonian of the statistical system, and the sum runs over all possible spin configurations and \( \beta = \frac{1}{k_B T} \), \( k_B \) being the Boltzmann constant.

If we transfer the similarities of the partition functions to the expectation values of observables, it gives

\[
\langle \hat{O}_{LAT} \rangle = \frac{1}{Z_G} \int \mathcal{D}[U] e^{-S_G[U]} \hat{O}_{LAT} \quad (1.70)
\]

and

\[
\langle \hat{O}_{STAT} \rangle = \frac{1}{Z_{STAT}} \sum_s e^{-\beta H[s]} \hat{O}_{STAT}. \quad (1.71)
\]

The displayed analogies between statistical mechanics and lattice gauge theory allows for the application of numerical methods developed for statistical mechanics(Chapter 1.3):

\[
\langle \hat{O} \rangle = \frac{1}{Z_G} \int \mathcal{D}[U] e^{-S_G[U]} O[U] = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} O[U_i], \quad (1.72)
\]
where the expectation values of operators are computed using the mean value of the functional $O[U_i]$ from $n$ gauge configurations $U_i$ (see (1.95)) distributed according to $P[U] = \frac{1}{Z_G} e^{-S_G[U]}$.

### 1.1.4. Lattice Gauge Theory at Finite Temperature

The similarities of a lattice gauge theory and statistical mechanics allow for the comparison of the partition functions of both systems.

$$Z_{LAT}(T) = tr \left[ e^{-aN_t \hat{H}} \right].$$  \hspace{1cm} (1.73)

The maximal time distance on the lattice is given by $aN_t$.

$$Z_{STAT}(T) = tr \left[ e^{-\beta \hat{H}} \right],$$  \hspace{1cm} (1.74)

where $\beta = \frac{1}{k_B T}$. The temperature is denoted by $T$ and the Boltzmann constant by $k_B$, $\hat{H}$ is the Hamiltonian of the quantum mechanical system. If we work with $k_B = 1$,

$$\beta = \frac{1}{T} = aN_t.$$  \hspace{1cm} (1.75)

This means that $aN_t$ has to be finite when the system is transferred to the continuum limit in order to keep the temperature of the system $T$ finite.
1.2. Finite Temperature Phase Transitions

Pure $SU(N)$ gauge theory exhibits a global symmetry, the so-called center symmetry. This symmetry is spontaneously broken when the system goes into the deconfined phase. This deconfinement phase transition of the pure $SU(N)$ gauge theory (at a critical temperature $T_c$) is related to the critical behaviour of an effective $Z_n$ spin model. This analogy (Svetitsky and Yaffe conjecture [11], [12]) allows for the realization of the pure $SU(3)$ gauge theory associated with QCD as an effective $Z_3$ spin model, a 3-state Potts model.

The QCD related model studied in this theory (in order to compare the outcome of different expansion techniques to existing data), is this effective $Z_3$ center model. Or being more specific, the confinement - deconfinement phase transition at finite temperature and finite chemical potential of this model is investigated.

An observable which distinguishes between the phase with broken symmetry and the phase where the center symmetry is intact has already been mentioned and is the so-called Polyakov loop.

In the following, we are going to introduce the center of a group and the center transformation, before we show how the Polyakov loop can be used as an order parameter. After that, we are going to review the Ising Model as an example for a system with a well defined order parameter (determining the phase transition and distinguishing between the center broken and the center symmetric phase) and as a special case of the Potts model.

1.2.1. Symmetry Transformations

The center $Z$ of a group $G$ is defined as

$$Z(G) = \{ z \in G | \forall g \in G, gz = zg \},$$

(1.76)

i.e. elements of the center commute with all elements of the group. The center of $SU(N)$ is denoted by $Z_N$. The $Z_N$ elements are given by

$$z_k = \exp i\Theta_k = \exp \left( \frac{i2\pi k}{N} \right),$$

(1.77)

with

$$k \in [0, 1, \cdots, N-1], \quad \Theta_k = \frac{2\pi k}{N}.$$

For $Z_3$, the center of the group $SU(3)$, these center elements are:

$$Z_3 = \left\{ 1, e^{i2\pi/3}, e^{-i2\pi/3} \right\}.$$
A center transformation of a gauge field can be defined in the following way

$$U_4(n, t_0) \rightarrow zU_4(n, t_0),$$  \hspace{1cm} (1.79)

where \( U_4(n, t_0) \) denotes temporal links in a given time slice \( n_4 = t_0 \) and \( z \) is a center element.

The plaquettes either do not contain the link \( U_\mu(n, t_0) \) at all or are invariant under center transformations (1.79):

$$\text{tr} \hspace{0.1cm} U_\mu(\mathbf{n}, t_0) \rightarrow \text{tr} \hspace{0.1cm} U_\mu(\mathbf{n}, t_0) = \left[ U_\mu(n, t_0)zU_4(n + \hat{\mu}, t_0)U_\mu(n, t_0) \right] \hspace{0.1cm} \left[ z^\dagger U_4(n, t_0)^\dagger \right]$$  \hspace{1cm} (1.80)

As a consequence, also the Wilson action is invariant under (1.79). The Haar measure (1.1.3) is invariant under center transformation as well [8]. However, the often mentioned Polyakov loop is an observable that is not invariant under center transformation.

1.2.2. The Polyakov Loop and the Center Transformation

The local Polyakov loop at \( \mathbf{m} \) is defined as

$$P(\mathbf{m}) = \text{tr} \left[ \prod_{j=0}^{N_t-1} U_4(m, j) \right].$$  \hspace{1cm} (1.81)

Under center transformation it transforms as

$$P \rightarrow zP.$$  \hspace{1cm} (1.82)

For the group \( SU(3) \), the Polyakov loop transforms under \( \mathbb{Z}_3 \) in the following way

$$\langle P \rangle = \frac{1}{3} \left( \sum_{i=1}^{3} z_i P \right) = \frac{1}{3} \left( 1 + e^{i2\pi/3} + e^{-i2\pi/3} \right) \langle P \rangle = 0,$$  \hspace{1cm} (1.83)

thus the only way to obtain a non vanishing \( \langle P \rangle \) is when the center symmetry is broken where in the second step it was assumed that \( \langle \ldots \rangle \) is invariant under center transformations.

The Polyakov loop is an important observable in pure gauge theory. It distinguishes between the deconfined phase with broken center symmetry and the confined phase where the center symmetry is intact. The useful properties of the Polyakov loop in pure gauge theory can be summarized as

$$\langle P \rangle = 0 \rightarrow \text{confined phase} \leftrightarrow \text{center symmetric phase}$$  \hspace{1cm} (1.84)

$$\langle P \rangle \neq 0 \rightarrow \text{deconfined phase} \leftrightarrow \text{center symmetry broken}$$  \hspace{1cm} (1.85)
1.2. Finite Temperature Phase Transitions

1.2.3. The Potts Model and Phase Transitions

In order to test the reliability of different expansion techniques in this work, we are going to investigate to which extent (concerning the chemical potential) the critical behaviour of a QCD related model can be reproduced. This means we are going to have a closer look at the phase transition of the system. We already mentioned, that this phase transition is closely related to the spontaneous breaking of the center symmetry. In this section, we are going to review an instructive spin model which gives an example for the relation of a phase transition to spontaneous symmetry breaking and is a special case of a Potts model at the same time, the two dimensional Ising model.

The Ising Model

The two dimensional Ising Model is a lattice spin model, where the spins can have the orientation \{+1, -1\} = Z_2. The spins are Z_2 elements in this manner (1.77). Below the critical temperature \(T_c\), all spins are parallel, leading to non-vanishing magnetization, whereas above the critical temperature, the spins point in arbitrary directions, leaving a vanishing magnetic moment. The magnetization can therefore be viewed as an order parameter of the Ising model, being zero above the critical temperature and non-vanishing below \(T_c\).

The interaction of the spins without an external magnetic field is determined by the Hamiltonian

\[
\hat{H} = -J \sum_{<i,j>} s_is_j,
\]

(1.86)

where \(J\) denotes the strength of the exchange interaction and the sum runs over the nearest neighbours. This model can be analyzed in terms of a Monte Carlo simulation, where configurations of the spins are produced according to their Boltzmann distribution (Chapter 1.3)

\[
P(S) \propto e^{-\beta H},
\]

(1.87)

where \(\beta\) denotes the inverse temperature. The average magnetization can be defined as

\[
M = \frac{1}{N} \sum_{i=1}^{N} s_i,
\]

(1.88)

where the sum runs over all lattice sites denoted \(i\) and \(N\) is the total number of sites. The order parameter \(M\) shows a second order phase transition at \(T_c\). It can also be noticed, that when the contributions of the spins cancel, \(M = 0\), the system is invariant under the transformation \(s_i \rightarrow -s_i\), which means \(M = 0\) in the symmetric phase. It is not difficult to imagine, that flipping the sign of the spins in the symmetry broken phase would lead to \(M \rightarrow -M\). \(M\) serves as an order parameter of the Ising model and distinguishes between the phase with broken center symmetry and the phase where the Z_2 symmetry of the Ising Model is intact.
1. Introduction

The Potts Model

Similar to the Ising model, the $q$-state Potts model consists of spins on a $d$ dimensional lattice, where the spins sit on the lattice sites $x$ and have directions according to a circle divided by $q$:

$$\Theta_x = \left\{ \frac{2\pi}{q}, \frac{4\pi}{q}, \ldots, 2\pi \right\} = \mathbb{Z}_q,$$

which is obviously equivalent to (1.77). The effective 3-dimensional $\mathbb{Z}_3$ model (at vanishing chemical potential) can be realized as a 3-state Potts Model in 3 dimensions. The phase transition of the system is going to be analyzed in terms of the Polyakov loop which serves as order parameter of the theory according to Section 1.2.2, where the chemical potential enters the theory via series expansion techniques.

![Spin orientations in a planar Potts model from [13].](image)

Similar to the Ising Model, also the Potts Model can be simulated numerically using the Monte Carlo approach. In the following section, this powerful numerical tool is introduced.

1.3. Simulation of Pure Gauge Theory

In 1.1.3 we mentioned, that physical quantities can be calculated using Euclidean correlators with methods from statistical mechanics 1.1.3 in the Monte Carlo approach. In this section, we give some basic details on Monte Carlo simulations.
1.3. Simulation of Pure Gauge Theory

The Euclidean correlators have already been expressed in terms of the path integral formalism. The expectation value of an arbitrary observable $O$ may be written as

$$\langle O \rangle = \frac{\int D[\Psi] O[\Psi] e^{-S_E[\Psi]}}{\int D[\Psi] e^{-S_E[\Psi]}}.$$  \hspace{1cm} (1.90)

Assuming the exponential is positive and real, the expectation value of $O$ is the average over all field configurations $\Psi$ of $O$, weighted with an exponential function that depends on the Euclidean action, $e^{-S_E[\Psi]}$. In principle, it is possible to calculate the expectation value of this arbitrary operator $O$, but one would have to average over infinitely many configurations! A way out would be the knowledge of the configurations which are to be expected and those which are very unlikely. This would allow for the neglect of the "less important" configurations, taking only into account some representative configurations.

1.3.1. Importance Sampling for Pure Gauge Theory

As less important configurations can be interpreted as highly unlikely configurations, we take probability theory into account and write the expectation value of the function $f(x)$ as

$$\langle f(x) \rangle = \frac{\int_a^b f(x) \rho(x) dx}{\int_a^b \rho(x) dx},$$  \hspace{1cm} (1.91)

where $\rho(x)$ is the density of the probability distribution. The expectation value $\langle f(x) \rangle$ can be approximated by

$$\langle f(x) \rangle_\rho = \frac{1}{N} \sum_{n=1}^{N} f(x_n),$$  \hspace{1cm} (1.92)

which is an average over $N$ values for $x_n \in (a, b)$, randomly sampled with the normalized probability density

$$dP(x) = \frac{\rho(x) dx}{\int_a^b \rho(x) dx}.$$  \hspace{1cm} (1.93)

The expectation value of an arbitrary observable $O$ for pure gauge theory on the lattice (in the path integral formalism) reads

$$\langle O \rangle = \frac{\int D[U] O[U] e^{-S_G[U]}}{\int D[U] e^{-S_G[U]}}.$$  \hspace{1cm} (1.94)

This is of the form (1.92) and can be written as

$$\langle O \rangle = \frac{1}{N} \sum_{n=1}^{N} O[U_n],$$  \hspace{1cm} (1.95)
where the $U[n]$ are sampled according to the Gibbs measure

$$dP(U) = \frac{e^{-S[U]}D[U]}{\int D[U]e^{-S[U]}}.$$  \hspace{1cm} (1.96)

The integral is now approximated by the sum over $N$ configurations where the $U_n$ are randomly sampled. In this manner, the statistical error is proportional to $1/\sqrt{N}$ and an exact value would be obtained from $N \rightarrow \infty$.

Importance sampling turns the integral over all possible configurations into a sum over the important configurations. An open question is, how we get from one configuration to the next.

1.3.2. Markov Chain

We are now going to follow subsequent configurations of the link variables $U_i$ in a so-called Markov process. The sequence of configurations is then called a Markov chain.

$$U_0 \rightarrow U_1 \rightarrow U_2 \rightarrow \cdots$$ \hspace{1cm} (1.97)

The transition from $U_i$ to $U_{i+1}$ is called a Markov step, or update. Figure [1.6] shows a schematic sketch of a Markov chain. The idea is to start at a random configuration (which may have a small probability density) and move along the Markov chain step-wise to configurations which are more important (center of Figure [1.6], meaning are more probable corresponding to their large Boltzmann factor $e^{-S}$). Observables are then evaluated when the system is in equilibrium, which means that the first Markov steps have to be discarded. In a Markov process, the configuration $U_i = U'$ is gen-

Figure 1.6: Schematic sketch of a Markov chain (1.97) connecting the subsequent configurations $U_i$ [8].
erated from the configuration $U_{i-1} = U$ by a random process which is defined by its transition probability

$$P(U_i = U' | U_{i-1} = U) = T(U'|U),$$  \hspace{1cm} (1.98)$$

which has to fulfil the two probability theoretical properties

$$0 \leq T(U' | U) \leq 1,$$  \hspace{1cm} (1.99)$$

and

$$\sum_{U'} T(U'|U) = 1.$$  \hspace{1cm} (1.100)$$

(1.99) means that the probability for a configuration to “occur” lies somewhere between zero and one, and that one of the configurations “happens” for sure (1.100). In order not to get ”stuck” at one point in the Markov chain, the probability to hop into a configuration $U_i$ has to be the same as to hop out of it. The corresponding balance equation

$$\sum_{U'} T(U'|U) P(U) = \sum_{U'} T(U'|U') P(U'),$$  \hspace{1cm} (1.101)$$

is solved by the term-wise holding equality

$$T(U'|U) P(U) = T(U'|U') P(U'),$$  \hspace{1cm} (1.102)$$

which is called the detailed balance condition. Furthermore, the Markov chain has to be strong ergodic, every configuration must be reachable within a finite number of Markov steps.

### 1.3.3. Metropolis Algorithm

The configurations in a Markov chain are subsequently visited according to their Boltzmann weight. Using the Metropolis algorithm, a Markov process transits from a state $U$ to a state $U'$ in the following way:

1. Suggest a new configuration $U'$ which is close to the old configuration $U$.

2. Calculate $\rho = P[U'|P[U] = \frac{e^{-S_G(U')}}{e^{-S_G(U)}}$.

3. Accept if $\rho \geq 1$ or if $\rho > r$, $r$ random number $\in [0, 1]$.


As an example, we consider the simulation of the $q$-state Potts model using the Monte Carlo method.
1. Introduction

Simulation of the Potts Model

The spin orientations $S_n \in \{1, 2, 3, \cdots, q\}$ give a $q$-state Potts model in $d$ dimensions with the Hamiltonian

$$H[S] = \alpha \sum_{n \in \Lambda} \sum_{\nu=1}^{d} [1 - \delta(S_n, S_{n+\nu})] + \mu \sum_{n \in \Lambda} [1 - \delta(S_n, 1)]. \tag{1.103}$$

Where $S$ denotes a configuration of spins, $\alpha$ is the next neighbour coupling strength and $\mu$ is an external magnetic field.

With

$$P[S] = e^{-\beta H[S]} \tag{1.104}$$

the Metropolis algorithm for the Potts model can be realized as:

1. Candidate configuration $S' \in \{1, 2, 3, \cdots, q\}$, randomly chosen
2. $\rho = P[S']/P[S] = e^{-\beta H[S']}/e^{-\beta H[S]}$, where only next neighbour interaction is considered
3. Accept if $\rho \geq 1$ or if $\rho > r$, $r$ random number $\in [0, 1]$.

The term "complex action problem" can be understood now: only a positive and real Boltzmann factor can be used as a probability weight. The action of the effective center model in its original form suffers from the complex action problem as well. For this reason, the 3-state Potts model in 3 dimensions representing the effective center model at vanishing chemical potential was simulated in this work. This was done with the purpose of inserting the outcome of the Potts model into three series expansion methods in order to evaluate observables at finite chemical potential. The first series expansion technique we are going to present is the fugacity expansion.
2. Fugacity Expansion

As already mentioned, the complex action problem has been solved for some theories in terms of so called dual variables. One of these theories is the effective center model, for which a phase diagram has been computed [7]. The results in terms of dual variables can be used to compare different expansion techniques for the $\mathbb{Z}_3$ model directly to the results obtained without any approximations. The first expansion technique to be studied is the fugacity expansion. For this purpose, the partition function will be rewritten to the Potts model representation of the $\mathbb{Z}_3$ spin model for vanishing chemical potential. This already enables one to compute the Polyakov loop and the corresponding susceptibility and hence to have a first look at the temperature dependence of the system, still at vanishing chemical potential. Also the expansion coefficients can be computed conveniently in the Potts model representation. The further steps are considerations about the convergence and the general behaviour of the coefficients of the fugacity series. After studying the temperature dependence of the analogues of the canonical determinants, observables for non vanishing chemical potential will be computed. The last step of this chapter will be the direct comparison of the calculated observables to results obtained in terms of dual variables for certain values of the chemical potential.

2.1. Fugacity Expansion in the $\mathbb{Z}_3$ Spin Model with Chemical Potential

Svetitsky and Yaffe pointed out that a confinement - deconfinement transition at finite temperature for the pure gauge group $SU(N)$ can be understood in terms of an effective scalar field theory with the same symmetry content [11], [12].

The Svetitsky - Yaffe conjecture allows for an effective theory for an order parameter which transforms under the center of the gauge group (which is a global symmetry group). The initial $d + 1$ dimensional gauge theory may be regarded as a $d$ dimensional spin system and the finite temperature transition in the gauge theory can be understood as an order - disorder transition in the effective model [11], [12].

For $SU(3)$, the gauge group of QCD, one can gather information about the deconfinement - transition by investigating the $\mathbb{Z}_3$ center group.

The $\mathbb{Z}_3$ model can be realised as a 3-state Potts model, where the Polyakov loops
2. Fugacity Expansion

can be thought of to be frozen to the center of the gauge group and where the order - disorder transition of the spin system gives insight into the confinement - deconfinement transition of the gauge theory, hence the Polyakov loop and the Potts model are said to be in the same universality class [13].

Furthermore, the leading effect of the fermions and their chemical potential can be taken into account by additional magnetic terms.

2.1.1. The Action of the Effective $\mathbb{Z}_3$ Model

Summarizing, at finite temperature the critical behaviour of $SU(3)$ gauge theory with additional terms from the fermions can be described via a $\mathbb{Z}_3$ spin model with the following effective action [14], [15], [16], [17]:

$$ S[P] = -\sum_x \left[ \tau \sum_{\nu=1}^{\beta} \left( P_x P^*_{x+\hat{\nu}} + c.c. \right) + \eta P_x + \bar{\eta} P^*_x \right]. $$

(2.1)

The degrees of freedom are given by the center variables $P_x \in \mathbb{Z}_3 = \{1, e^{i \frac{2\pi}{3}}, e^{-i \frac{2\pi}{3}}\}$, which sit on the sites of a three dimensional lattice with periodic boundary conditions and correspond to local Polyakov loops. In (2.1) $\hat{\nu}$ is a unit vector pointing in all directions of the three-dimensional lattice. The parameter $\tau$ is identified with an increasing function of the temperature in the derivation of (2.1) and will be referred to as temperature hereafter. The chemical potential $\mu$ enters the action via

$$ \eta = \kappa e^{\mu}, $$

$$ \bar{\eta} = \kappa e^{-\mu}, $$

where $\kappa$ increases with decreasing quark mass and is proportional to the number of flavours.

As already mentioned, we want to calculate observables, like the internal energy, in this chapter. That means we need the partition function of the system. Since we are now familiar with the action of the model in consideration, we can write

$$ Z = \sum_{\{P\}} e^{-S[P]}, $$

(2.2)

The partition function is a sum over the configurations of the center elements sitting on the lattice sites.
2.1. Fugacity Expansion in the $Z_3$ Spin Model with Chemical Potential

2.1.2. The Order Parameter

A very important observable is the Polyakov loop, which can be defined as

$$\langle P \rangle = \left\langle \frac{1}{N^3} \sum_x P_x \right\rangle,$$  \hspace{1cm} (2.3)

and serves as an order parameter of the theory, where $N^3$ is the total number of sites of our 3-dimensional lattice.

We already introduced the Polyakov loop as an order parameter in Section 1.2.2 with (1.84) and (1.85):

$$\langle P \rangle = 0 \rightarrow \text{confined phase} \leftrightarrow \text{center symmetric phase} \hspace{1cm} (2.4)$$

$$\langle P \rangle \neq 0 \rightarrow \text{deconfined phase} \leftrightarrow \text{center symmetry broken} \hspace{1cm} (2.5)$$

Equation (2.3) reveals the order-disorder distinction of the Polyakov loop immediately. (2.3) tells us to sum over all spins, divide by the number of lattice points and average over a number of configurations for the evaluation of the Polyakov loop expectation value. The analogy to the magnetization (1.88) in the Ising model reviewed in 1.2.3 is obvious. $\langle P \rangle = 0$ when the spins on the lattice are randomly oriented and therefore cancel, implying invariance of $\langle P \rangle$ under exchange of the sign of the center elements. The system is in the symmetric phase. If $\langle P \rangle \neq 0$ the $Z_3$ symmetry is broken.

As mentioned above, the order - disorder transition corresponds to the confinement - deconfinement transition of the theory.

Having introduced the action, partition sum and order parameter of the system, we are now going to consider the fugacity expansion.

2.1.3. The Fugacity Expansion

The fugacity expansion is an expansion of the partition sum in terms of the fugacity parameter $e^{\mu}$:

$$Z(\mu) = \sum_{q \in \mathbb{Z}} e^{\mu q} Z_q,$$  \hspace{1cm} (2.6)

where $q$ runs over all net quark numbers.

The chemical potential $\mu$ can be replaced by an imaginary chemical potential $\mu = i\varphi$

$$Z(i\varphi) = \sum_{q \in \mathbb{Z}} e^{i\varphi q} Z_q.$$  \hspace{1cm} (2.7)
Fourier transformation with respect to $\phi$ gives

$$
\frac{1}{2\pi} \int_{-\pi}^{\pi} Z(\epsilon \phi) e^{-i\epsilon \phi} d\phi = \sum_{q} Z_q \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\epsilon (q-q')} d\phi = Z_q.
$$

$Z_q$ can furthermore be written as follows:

$$
Z_q = \frac{1}{2\pi} \int_{-\pi}^{\pi} Z(\epsilon \phi) e^{-i\epsilon \phi} d\phi \\
= \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{\{P\}} \exp \left\{ \sum_{x} \left[ \tau \cdot \sum_{\nu=1}^{3} [P_x \cdot P_{x+\nu}^* + c.c.] + \kappa e^{i\epsilon P_x} + \kappa e^{-i\epsilon P_x^*} \right] \right\} e^{-i\epsilon \phi} d\phi \\
= \sum_{\{P\}} \exp \left\{ \sum_{x} \left[ \tau \cdot \sum_{\nu=1}^{3} [P_x \cdot P_{x+\nu}^* + c.c.] \right] \right\} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\epsilon \phi} \exp \left\{ \kappa e^{i\epsilon \sum_{x} [P_x + \kappa e^{-i\epsilon} \sum_{x} P_x^*] \right\}.
$$

As the sum over $P_x$ is a complex quantity, one can define

$$
\sum_{x} P_x \equiv R[P] \cdot e^{i\theta[P]} \equiv H,
$$

and $Z_q$ is then given by

$$
Z_q = \sum_{\{P\}} e^{i\epsilon \sum_{x,\nu} [P_x \cdot P_{x+\nu}^* + c.c.]} D_q[P], \quad (2.9)
$$

were the $D_q[P]$ are given by

$$
D_q[P] = \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{-i\epsilon \phi} \exp \left\{ \kappa \left[ e^{i(\phi + \theta[P])} + e^{-i(\phi + \theta[P])} \right] \right\} R[P], \\
= e^{i\theta[P]} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \exp \left\{ 2\kappa \cos \phi R[P] \right\} e^{-i\epsilon \phi}.
$$

Here, the new angle $\phi + \theta[P] = \phi'$ has been introduced. We obtain for the $D_q[P]$:

$$
D_q[P] = e^{i\theta[P]} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \exp \left\{ 2\kappa \cos \phi R[P] \right\} e^{-i\epsilon \phi} \\
= e^{i\theta[P]} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} \exp \left\{ 2\kappa \cos \phi R[P] \right\} \cos (\phi t_q).
$$

Comparison with the regular modified cylindric Bessel functions

$$
I_n(P) = \frac{1}{\pi} \int_{0}^{\pi} d\phi e^{\epsilon \cos \phi} \cos (n\phi),
$$

determines the $D_q$ consequentially as

$$
D_q[P] = e^{i\theta[P]} \cdot I_q(2\kappa R[P]). \quad (2.10)
$$
2.1. Fugacity Expansion in the $\mathbb{Z}_3$ Spin Model with Chemical Potential

An alternative expression for the partition function is

$$Z_q = \sum_{\{P\}} e^{\tau \sum_{x,\nu} [P_x + P^*_x + \chi.c.c.] + \kappa \sum_x [P_x + P^*_x]} \cdot \tilde{D}_q,$$

with

$$\tilde{D}_q = e^{i\theta_i |q| I_q} (2\kappa R [P]) \cdot e^{-\kappa \sum_x [P_x + P^*_x]}.$$  \hspace{1cm} (2.11)

### 2.1.4. Observables Related to the Particle Number

As it is one purpose of this work to evaluate observables using the fugacity expansion, a first look at their calculation is taken. For example, observables related to the particle number can be derived from the fugacity expansion and assume a particularly simple form. The expectation value of the particle number reads

$$\langle q \rangle = \frac{\partial}{\partial \mu} \ln Z(\mu) = \frac{\sum_q q \cdot e^{\mu q} \cdot \langle \tilde{D}_q \rangle_0}{\sum_q e^{\mu q} \cdot \langle \tilde{D}_q \rangle_0} = \frac{\langle M_1 \rangle_0}{\langle M_0 \rangle_0},$$  \hspace{1cm} (2.13)

where the moments $M_n$ are defined as

$$M_n = \sum_q q^n e^{\mu q} \tilde{D}_q.$$  \hspace{1cm} (2.14)

The expectation value of the ensemble in (2.13) is understood to be calculated at zero chemical potential, $\langle X \rangle_0 = \frac{1}{Z_0} \sum_{\{P\}} e^{-S_0} X$.

In the same way, the particle number susceptibility is given by

$$\chi_q = \frac{\partial^2}{\partial \mu^2} \ln Z(\mu) = \frac{\langle M_2 \rangle_0}{\langle M_0 \rangle_0} - \left( \frac{\langle M_1 \rangle_0}{\langle M_0 \rangle_0} \right)^2.$$  \hspace{1cm} (2.15)

For the numerical evaluation of $\langle M_n \rangle_0$ it is convenient to map the model to a Potts model representation which is possible at $\mu = 0$. 

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2. Fugacity Expansion

2.2. Potts Model Representation of the Effective Center Model at $\mu = 0$

To simulate the $Z_3$ spin model, one has to find an optimal representation of the partition sum at vanishing chemical potential, this is what will be done in the following.

The spin variables can be parameterized as

$$ P_x = e^{i \frac{2\pi}{3} n_x}, \quad (2.16) $$

with

$$ n_x \in \{-1, 0, 1\}. $$

The partition function in the case of vanishing chemical potential then reads

$$ Z_{\mu=0} = \sum_{\{n\}} \exp \left\{ \tau \sum_{x,\nu} \left[ e^{i \frac{2\pi}{3} n_x} \cdot e^{-i \frac{2\pi}{3} n_{x+\hat{\nu}}} + \text{c.c.} \right] \right\} \exp \left\{ \kappa \sum_x \left[ e^{i \frac{2\pi}{3} n_x} + e^{-i \frac{2\pi}{3} n_x} \right] \right\}, $$

where the first sum runs over all configurations of the $n_x$. Therefore

$$ Z_{\mu=0} = \sum_{\{n\}} \prod_{x,\nu} e^{2\tau \cos \left( \frac{2\pi}{3} (n_x - n_{x+\hat{\nu}}) \right)} \cdot \prod_x e^{2\kappa \cos \left( \frac{2\pi}{3} n_x \right)}, $$

Since

$$ \cos \left( \frac{2\pi}{3} |n_x - n_{x+\hat{\nu}}| \right) = \begin{cases} 1 & \text{if } n_x = n_{x+\hat{\nu}}, \\ -\frac{1}{2} & \text{if } n_x \neq n_{x+\hat{\nu}}, \end{cases} $$

the partition can be written as

$$ Z_{\mu=0} = \sum_{\{n\}} \exp \left\{ 3\tau \sum_{x,\nu} \delta_{n_x,n_{x+\hat{\nu}}} + 3\kappa \sum_x \delta_{n_x,0} \right\}. \quad (2.17) $$

Equation $(2.17)$ is the representation of the $\mu = 0$ - partition sum as a Potts model, which we use for the simulation of the $Z_3$ model in the Monte Carlo approach (Chapter 1.3).
2.2. First Observations: Polyakov Loop and Polyakov Loop Susceptibility

As it is already possible to calculate the Polyakov loop expectation value defined in (2.3) this observable can be used for two purposes. Firstly, we can inspect the correctness of the Potts model simulation by comparing the results for the Polyakov loop of our model directly to results in terms of dual variables for different values of $\kappa$ (Figure 2.1). The coloured lines are those of the dual variable results [7], whereas the black lines with errorbars correspond to results of our Potts model simulation. Due to the fact that the results coincide as they should, errorbars are not shown for the dual variable data.

However, the main attraction of this graph is the possibility to observe the phase transition of the system. It is known that the effective center model undergoes a first order phase transition for very small values of $\kappa$ and vanishing chemical potential until a critical end point $(\tau_c, \kappa_c = [0.183127(7), 0.00026(3)])$ [18], [19], [20], whereas for larger $\kappa$ the transition is considered to be a crossover [7]. Figure 2.1 confirms these facts: only for $\kappa < \kappa_c$ the Polyakov loop data start to resemble the discontinous behaviour of a first order transition (a true transition is of course only possible for infinite volume). As mentioned in Section 2.1 the Polyakov loop serves as order parameter of the theory.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.1.png}
\caption{Comparison of the Polyakov loop as a function of temperature (black) for 7 different values of $\kappa$ to results in terms of dual variables (coloured) [7] for $10^6$ measurements on a $16^3$ lattice.}
\end{figure}
2. Fugacity Expansion

Starting the analysis with the smallest value of $\kappa$, the inverse mass parameter, one can observe the expected symmetric phase at small temperatures, where the expectation value of the Polyakov loop is very close to zero (since $\langle |P| \rangle$ suffers from finite size effects). Increasing the temperature leads the system into a phase with broken symmetry, where the order parameter assumes finite values. For $\kappa = 0.001$, the rapidity of the transition with respect to temperature can be clearly seen and a first order phase transition can be presumed.

This is corroborated by the examination of the derivative of the logarithm of the partition function with respect to $\eta$, the Polyakov loop susceptibility. The Polyakov loop susceptibility (Figure 2.2) which, in the case of vanishing chemical potential, is given by

$$\chi_P = \langle H^2 \rangle_0 - \langle H \rangle_0^2,$$

(2.18)

can already be calculated from the Potts model data ($H = \sum_x P_x$).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig22.png}
\caption{Comparison of the Polyakov loop susceptibility as a function of temperature (black) for 7 different values of $\kappa$ to results in terms of dual variables (coloured) for 10^6 measurements on a 16^3 lattice.}
\end{figure}

Figure 2.2 shows the Polyakov loop susceptibility for different values of $\kappa$. The pronounced peak for $\kappa = 0.001$ is again an indication for a first order transition, which can be confirmed by the finite volume scaling behaviour of $\chi_P$.

If the Polyakov loop susceptibilities diverge proportional to the volume, the phase transition is of first order.
Volume scaling can be seen in Figure 2.3(a) for a very small value of $\kappa$, whereas higher values of $\kappa$ do not show this dependence on the volume of the lattice (Figure 2.3(b)), showing that there only a crossover takes place.

**Figure 2.3.** Finite volume scaling behaviour of $\chi_P$ as a function of temperature for different lattice sizes $N$ for $\kappa = 0.001$ and $\kappa = 0.05$. 
2.3. Convergence of the Fugacity Series

Since it is not possible to compute the full fugacity sum given by (2.6), the sum has to be truncated, and some considerations about the convergence of the fugacity series have to be made.

For this purpose we inspect the equality of (2.2) and (2.6), both equations describing the partition sum. Hence

\[
Z = \sum_{\{P\}} e^{-S[P]} = \sum_{\{P\}} e^{\sum_{x} \left[ \tau \sum_{x,v=1}^{3} \left( P_{x} + P_{x+\hat{v}} + c.c. \right) + \eta P_{x} + \bar{\eta} P_{x}^{*} \right]}
\]

\[
= \sum_{\{P\}} e^{\tau \sum_{x,v=1}^{3} \left[ P_{x} P_{x+\hat{v}} + c.c. \right]} \cdot e^{\sum_{x} \left[ \eta P_{x} + \bar{\eta} P_{x}^{*} \right]}
\]

\[
= \sum_{q} e^{\mu q} Z_{q}
\]

\[
= \sum_{q} e^{\mu q} \left( \sum_{\{P\}} e^{\tau \sum_{x,v=1}^{3} \left[ P_{x} P_{x+\hat{v}} + c.c. \right]} \cdot D_{q} [P] \right).
\]

This yields the equation:

\[
\sum_{\{P\}} e^{\sum_{x} \left[ \eta P_{x} + \bar{\eta} P_{x}^{*} \right]} = \sum_{q} e^{\mu q} \cdot \sum_{\{P\}} D_{q} [P],
\]

(2.19)

where the left hand side is the part of the Boltzmann factor depending on the chemical potential and the right hand side is the corresponding fugacity expansion.

Therefore the relative error, referred to as \( \Delta \), can be obtained as:

\[
\Delta = \frac{|L - R|}{|L|}.
\]

(2.20)

We have found a quantity which is sensitive to the choice of the lower \( q_{l} \) and upper \( q_{u} \) cut values of our truncated fugacity series

\[
Z_{\text{trunc}} = \sum_{q=q_{l}}^{q_{u}} e^{\mu q} Z_{q}.
\]

(2.21)

Nevertheless, one has to know something about the behaviour of the contributions of the coefficients in the fugacity sum to find the right \( q_{\text{cut}} \) (\( q_{l} \) and \( q_{u} \)) without guesswork.
2.3. Convergence of the Fugacity Series

2.3.1. Coefficients of the Fugacity Sum at $\mu = 0$

As it is not possible to compute the full sum over $q$ in (2.6), one has to investigate a truncated sum from a certain $q_l$ to a distinct upper $q_u$, this means one has to find the coefficients of the fugacity sum that have a sizable contribution.

It is possible to gain insight into the behaviour of the coefficients already at vanishing chemical potential, this is what will be done first. Afterwards, the coefficients of the fugacity series will be analyzed for finite chemical potential, which essentially amounts to a shift of their relative weight.

In case of $\mu = 0$, one can find the coefficients of the fugacity sum that have a sizable contribution by plotting the mean of the absolute value of $D_q$ normalized by $D_0$ as a function of $q$. Figure 2.4 shows such a distribution of the $D_q$ for different values of the temperature. From Figure 2.4 it can be seen, that the $D_q$ have a distribution that

![Figure 2.4](image)

Figure 2.4.: $\langle |D_q|/D_0 \rangle$ as function of $q$ for various values of $\tau$; $\tau_{\text{crit}} \simeq 0.182$; $\mu = 0$ on a $16^3$ lattice for $\kappa = 0.001$.

resembles a Gaussian, and that for vanishing chemical potential, the bell curve is symmetric with respect to the origin. Furthermore increasing the temperature broadens the distribution, leading to higher values of $q_{\text{cut}}$.
2. Fugacity Expansion

The susceptibility $\chi_q$ is related to the second moment of the $D_q$ which is proportional to the width of the distribution. From Figure 2.4 follows, that $\chi_q$ increases with temperature. At $\tau_c = 0.182$ a strong increase in the susceptibility $\chi_q$ can be expected. A comparison with Figure 2.10 confirms this.

It was already found that the susceptibility $\chi_q$ is related to the second moment of the $D_q$, which is proportional to the width of the distribution. Since $\chi_q$ is an extensive quantity, the width of the distribution should also grow with the volume.

Modelling the distribution of the $D_q$ by a Gaussian one finds

$$\chi_q = \frac{\partial^2}{\partial \mu^2} \ln Z = \frac{1}{Z} \sum_q e^{\frac{-q^2}{2\sigma^2}} \cdot e^{\mu q}$$

$$= \left( \sum_q e^{\frac{-q^2}{2\sigma^2}} \cdot e^{\mu q} \cdot q^2 \right)^2$$

$$= \left( \langle q^2 \rangle - \langle q \rangle^2 \right) \bigg|_{\mu=0} = \langle q^2 \rangle.$$ 

The sum can be approximated by an integral

$$\chi_q \simeq \frac{1}{Z} \sum_q e^{\frac{-q^2}{2\sigma^2}} \cdot q^2 \simeq \frac{1}{Z} \int_{-\infty}^{\infty} e^{\frac{-q^2}{2\sigma^2}} \cdot q^2 dq.$$ 

The same step for the partition sum gives:

$$Z \simeq \sum_q e^{\frac{-q^2}{2\sigma^2}} \simeq \int_{-\infty}^{\infty} e^{\frac{-q^2}{2\sigma^2}} dq.$$ 

A transformation of variables

$$p = \frac{q}{\sigma},$$

gives the result

$$\chi_q \simeq \frac{\sigma^3 \cdot \int_{-\infty}^{\infty} e^{\frac{p^2}{2\sigma^2}} dp \cdot p^2 dp}{\sigma \cdot \int_{-\infty}^{\infty} e^{\frac{p^2}{2\sigma^2}} dp} \simeq \sigma^2 \cdot \text{const.}.$$ 

And thus we find

$$\sigma^2 = \frac{\chi_q}{\text{const.}} = A \cdot V \rightarrow \sigma \sim \sqrt{V}. \quad (2.22)$$

This implies that the width of the distribution scales like the square root of the volume. A careful inspection of Figure 2.5 shows that this law is approximately seen in our data.
2.3. Convergence of the Fugacity Series

Figure 2.5.: Distribution of the coefficients of the fugacity series for vanishing chemical potential for $\kappa = 0.001$ and 4 different values of $\tau$ ($a, b, c, d$) for lattice sizes $N^3$ with $N = 8, 12, 16$ in each case.
2. Fugacity Expansion

2.3.2. Coefficients of the Fugacity Expansion at Finite Chemical Potential

When the chemical potential is activated, it enters the fugacity series via the factor $e^{\mu q}$. The result of the competition of this exponentially increasing term and the $D_q$ with their Gaussian-like distribution, can be studied by plotting the expectation value of the absolute value of $D_q$ times $e^{\mu q}$ normalized by $D_0$.

\[ \langle |D_q e^{\mu q}| / D_0 \rangle \]

**Figure 2.6.** $\langle |D_q e^{\mu q}| / D_0 \rangle$ for different values of $\mu$, $\kappa = 0.001$, $\tau = 0.183$ on a $16^3$ lattice.

From Figure 2.6 it can be seen how the distribution grows with increasing chemical potential and how it moves to higher values of $q$, abandoning the symmetry with respect to the origin. This is exactly what the chemical potential is expected to do: it shifts the means of the distribution towards non-zero values of $q$.

The important technical consequence of this shift is that the boundaries of the truncated sum of the fugacity expansion must be adapted, since the contributions $e^{\mu q}D_q$ are shifted towards higher values of $q$.

In summary it can be concluded that $q_l$ and $q_u$ depend on $\tau$, $\kappa$, $\mu$ and on the lattice size $N$. 
2.3. Convergence of the Fugacity Series

To stress and visualize this important point, Figure 2.7 shows the distributions of the coefficients in the fugacity expansion for temperatures above and below the phase transition for two values of $\kappa$.

![Figure 2.7](image_url)

**Figure 2.7.** Distribution of the coefficients of the fugacity series as function of $q$ for various values of the chemical potential for $\kappa = 0.001$ and $\kappa = 0.01$. Shown are 2 values of $\tau$ for lattice size $16^3$.

From Figure 2.7 it can be observed, that a few values of $q$ are sufficient for the fugacity expansion to converge in the case of $\kappa = 0.001$, whereas for $\kappa = 0.01$ $q_{cut}$ is remarkably higher. This leads to very high orders of Bessel functions with small arguments to be computed.

The fugacity series is more difficult to be calculated for small values of $\kappa$. A reason for this will be given in Chapter 3.
2.3.3. Relative Error

Although the distribution of the coefficients in the fugacity sum is helpful to identify $q_{cut}$, a serious analysis of convergence requires the careful study of $\Delta$. Figure 2.8 (top) shows an example of the sensitivity of $\Delta$ regarding $q_{cut}$ for three scenarios where the fugacity sum is too rigorously truncated from below (red), $q_u$ is too small (green) and the case of a reasonable truncated sum (blue), leading to a very small error for the whole range of the chemical potential. For the case of higher $\kappa$ (Figure 2.8 (bottom)) $q_{cut}$ has to be increased to minimize $\Delta$, in agreement with Figure 2.7.

Figure 2.8.: Relative error $\Delta$ as function of the chemical potential for $\kappa = 0.001$ and $\tau = 0.1965$ on a $16^3$ lattice for three combinations of $q_{cut}$ (top), Relative error $\Delta$ as function of the chemical potential for $\kappa = 0.01$ and $\tau = 0.16$ on a $16^3$ lattice (bottom).
2.4. Scatter Plots of the Canonical Determinants

Properties of canonical determinants are analyzed in [21], where they are coefficients in a fugacity expansion of the grand canonical determinant. One property of these coefficients is their distinction between the center symmetric phase and the phase with broken center symmetry, which can be observed via scatter plots. Furthermore, the canonical determinants analyzed in [21] scatter isotropically around the origin when the system is in the symmetric phase, whereas they form a distinctive pattern - familiar from the Polyakov loop - when the system is in the phase with broken center symmetry [22], [21]. In our theory, the quantities corresponding to the canonical determinants are the $\tilde{D}_q$, given by (2.12). Thus it is interesting to investigate, if scatter plots of the $\tilde{D}_q$ also show specific patterns in distinctive phases. From Figure 2.9 it can be seen,

that the analogues of the canonical determinants in our theory distinguish between the symmetric phase and the phase with broken symmetry. However, they do not show specific patterns above the critical temperature.

Figure 2.9.: Scatter Plots of $\tilde{D}_q$ in the complex plane for the critical temperature $\tau_c = 0.182$ (center), $\tau = 0.16$ (top) and $\tau = 0.1905$ (bottom). Note that the scales of the plots are chosen differently.
2.5. Observables in the Fugacity Expansion

The following chapter is dedicated to the calculation of observables using the fugacity expansion. The first part of this chapter deals with the two observables quark number and internal energy and the corresponding two susceptibilities at zero chemical potential. Thereafter the same observables and the Polyakov loop with its susceptibility are evaluated for finite chemical potential. The results are discussed and compared to flux representation results for certain values of chemical potential.

2.5.1. Observables at $\mu = 0$

We begin with observables at vanishing chemical potential. This will give some further insight into the model under consideration and allows for consistency checks, before the analysis of observables for finite chemical potential.

Polyakov Loop and Polyakov Loop Susceptibility

The Polyakov loop and the Polyakov loop susceptibility were already discussed in Section 2.2.1.

Quark Number and Quark Number Susceptibility

For a system without chemical potential, the expectation value of the particle number vanishes. The quark number susceptibility, however, is non-zero.

For $\mu = 0$, there are 2 possibilities to calculate the quark number susceptibility. The first one can be derived from (2.15):

$$\chi_q = 1 \cdot \sum_q \langle \tilde{D}_q \rangle \cdot q^2,$$

(2.23)

where

$$Z = \sum_q \langle \tilde{D}_q \rangle.$$

The second method to get $\chi_q$ is to work in the conventional representation and to evaluate the definition

$$\chi_q \bigg|_{\mu=0} \simeq \frac{1}{V} \frac{\partial^2 \ln Z}{\partial \mu^2} \bigg|_{\mu=0}.$$

(2.24)
One finds
\[
\chi \bigg|_{\mu = 0} = \frac{1}{V} \left( \frac{\partial S}{\partial \mu} \right)_{\mu = 0} = \kappa \cdot 2 \cdot i \cdot \Im(H).
\]
\[
-\frac{\partial^2 S}{\partial \mu^2} \bigg|_{\mu = 0} = \kappa \cdot 2 \cdot \Re(H).
\]
And thus
\[
\chi_q \bigg|_{\mu = 0} = \frac{1}{V} \left[ -4\kappa \langle [\Im(H) - \langle \Im(H) \rangle]^2 \rangle + 2\kappa \langle \Re(H) \rangle \right] .
\]
\[
\chi_q \bigg|_{\mu = 0} = \frac{1}{V} \left[ -4\kappa^2 \langle \Im(H)^2 \rangle + 2\kappa \langle \Re(H) \rangle \right] .
\] (2.25)

The two ways of evaluating \( \chi_q \) should give the same results and a comparison of the two methods (Figure 2.10) is therefore an important consistency check. Also the aforementioned temperature dependence of \( \chi_q \), observed in Figure 2.4, is confirmed.
2. Fugacity Expansion

The last investigated observables for vanishing chemical potential are the internal energy and the corresponding susceptibility, the heat capacity. Using fugacity expansion, they assume the form

\[ U = \frac{\sum_q \langle \tilde{D}_q \cdot S_\mu \rangle_0}{\sum_q \langle \tilde{D}_q \rangle_0}, \quad (2.26) \]

\[ C = \langle S^2 \rangle_\mu - \langle S \rangle_\mu^2 = \frac{\sum_q \langle \tilde{D}_q S^2 \rangle_0}{\sum_q \langle \tilde{D}_q \rangle_0} - \left( \frac{\sum_q \langle \tilde{D}_q S \rangle_0}{\sum_q \langle \tilde{D}_q \rangle_0} \right)^2. \quad (2.27) \]

The following graphs show the internal energy (2.26) and the heat capacity (2.27) at vanishing chemical potential for two values of \( \kappa \).

Figure 2.10.: Comparison of \( \chi_q \) obtained as derivative of the partition sum (\( Z \)) and as in (2.23) (\( D_q \)) as function of temperature for \( \kappa = 0.001 \) on a 16\(^3\) lattice.
It is expected, that the system lowers its energy, when it transitions into the phase with broken symmetry. Figure 2.11 confirms this prediction.

Figure 2.11.: Internal energy $U$ as a function of temperature for $\kappa = 0.001$ (l.h.s.) and $\kappa = 0.01$ (r.h.s.) at $\mu = 0$ on a $16^3$ lattice for $10^6$ measurements. For $\kappa = 0.001$ $q_l = q_u = 30$ and for $\kappa = 0.01$ $q_l = 25$ and $q_u = 85$.

Figure 2.12.: Heat capacity $C$ as a function of temperature for $\kappa = 0.001$ (l.h.s.) and $\kappa = 0.01$ (r.h.s.) at $\mu = 0$ on a $16^3$ lattice for $10^6$ measurements. For $\kappa = 0.001$ $q_l = q_u = 30$ and for $\kappa = 0.01$ $q_l = 25$ and $q_u = 85$.

The critical temperature is marked by the maximum of the heat capacity of the system, shown in Figure 2.12. Since the positions of the peaks of heat capacity and Polyakov loop susceptibility do not coincide for $\kappa = 0.01$, the crossover nature of the phase transition is again confirmed.
2. Fugacity Expansion

2.5.2. Observables at $\mu \neq 0$

While the first part of this section dealt mostly with consistency checks, the second part will be devoted to bypass the complex action problem to a certain degree using fugacity expansion techniques and observables at finite chemical potential.

Polyakov Loop and Polyakov Loop Susceptibility

The Polyakov loop is given by the derivative of the logarithm of the partition function with respect to $\eta$

$$\langle P \rangle_\mu = \frac{\partial}{\partial \eta} \ln Z(\mu) = \frac{1}{Z(\mu)} \cdot \sum_P e^{-S[P]} \cdot H = \langle H \rangle_\mu,$$

(2.28)

where $H$ is again defined as in [2.8]. The corresponding susceptibility $\chi_P$ is obtained as second derivative of the logarithm of the partition function with respect to $\eta$

$$\chi_P = \langle H^2 \rangle_\mu - \langle H \rangle_\mu^2.$$

(2.29)

Since the Potts model representation only allows for the evaluation of expectation values at vanishing chemical potential, we are now going to use the fugacity expansion to derive an expression for $\langle H^n \rangle_\mu$ where only expectation values at $\mu = 0$ are needed.

$$\langle H^n \rangle_\mu = \frac{1}{Z(\mu)} \sum_{\{P\}} e^{-S[P]} H[P]^n = \frac{1}{Z(\mu)} \sum_{\{P\}} e^{-S_0} \sum_q e^{\mu q} \tilde{D}_q[P] \cdot H[P]^n$$

$$= \sum_q e^{\mu q} \frac{1}{Z(\mu)} \sum_{\{P\}} e^{-S_0} \tilde{D}_q[P] \cdot H[P]^n = \sum_q e^{\mu q} \frac{Z_0}{Z_\mu} \langle \tilde{D}_q H^n \rangle_0$$

$$= \sum_q e^{\mu q} \langle \tilde{D}_q \cdot H^n \rangle_0.$$

Thus we find for the Polyakov loop and the corresponding susceptibility in the fugacity expansion formulation

$$\langle P \rangle_\mu = \frac{\sum_q e^{\mu q} \langle \tilde{D}_q \cdot H \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0},$$

(2.30)

$$\chi_P = \frac{\sum_q e^{\mu q} \langle \tilde{D}_q \cdot H^2 \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0} - \left( \frac{\sum_q e^{\mu q} \langle \tilde{D}_q \cdot H \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0} \right)^2.$$

(2.31)

The preceding calculation allows for the computation of the Polyakov loop and the Polyakov loop susceptibility at non-vanishing chemical potential. We show how the observables in question change with the chemical potential for 2 values of $\kappa$ and for $\mu$ up to 1 in the vicinity of the critical temperature.
2.5. Observables in the Fugacity Expansion

Figure 2.13: Polyakov loop as function of temperature for $\kappa = 0.01$ (top) and $\kappa = 0.001$ (bottom) on a $16^3$ lattice for various values of $\mu$. The data is from $10^6$ measurements. For $\kappa = 0.01 \ q_l = 25, q_u = 85$ for $\mu \leq 0.8; q_u = 130$ for $\mu = 0.9; q_u = 132$ for $\mu = 1.0$ and for $\kappa = 0.001 \ q_l = q_u = 30$ for $\mu \leq 0.5$ whereas $q_l = 20, q_u = 40$ for $\mu > 0.5$. 

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Figure 2.14.: Polyakov loop susceptibility as function of temperature for $\kappa = 0.01$ (top) and $\kappa = 0.001$ (bottom) for various values of $\mu$ on a $16^3$ lattice obtained from $10^6$ measurements. The $q_{cut}$ are chosen corresponding to those of the Polyakov loop.
2.5. Observables in the Fugacity Expansion

Figure 2.13 shows that the phase transition of the system softens as the chemical potential is increased. This fact can also be seen in the graph of the second derivative of the logarithm of the partition function with respect to \( \eta \) (Figure 2.14). Moreover, Figure 2.14 illustrates how the critical temperature decreases with increasing chemical potential.

Since the complex action problem is more dominant for higher values of the inverse mass parameter \( \kappa \), thus for smaller particle masses (as will be shown in Chapter 3), the kink in the Polyakov loop near the phase transition for \( \mu = 1 \) results in a larger error in its derivative. Therefore only values for \( \mu \) up to 0.8 are shown for \( \kappa = 0.01 \).

Quark Number and Quark Number Susceptibility

In the same way, as the Polyakov loop and the Polykov loop susceptibility were evaluated, also the quark number and the quark number susceptibility can be derived easily using the fugacity expansion.

The particle number reads

\[
\langle q \rangle = \frac{\sum_q q \cdot e^{\mu q} \cdot \langle \tilde{D}_q \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0}.
\]

(2.32)

It is convenient to introduce the moments \( M_n \) defined as

\[
\langle M_n \rangle_0 = \sum_q q^n e^{\mu q} \langle \tilde{D}_q \rangle_0.
\]

(2.33)

Hence

\[
\langle q \rangle = \frac{\langle M_1 \rangle_0}{\langle M_0 \rangle_0},
\]

(2.34)

and

\[
\chi_q = \frac{\langle M_2 \rangle_0}{\langle M_0 \rangle_0} - \left( \frac{\langle M_1 \rangle_0}{\langle M_0 \rangle_0} \right)^2.
\]

(2.35)

As the particle number is very sensitive to chemical potential, graphs for \( \mu \) up to 0.5 are shown for two values of \( \kappa \).
2. Fugacity Expansion

Figure 2.15.: Particle number as function of temperature at $\kappa = 0.01$ (top) and at $\kappa = 0.001$ (bottom) on a $16^3$ lattice ($10^6$ measurements).
Figure 2.16.: Particle number susceptibility as function of temperature at $\kappa = 0.01$ (top) and at $\kappa = 0.001$ (bottom) on a $16^3$ lattice ($10^6$ measurements).
Figure 2.15 shows how the system reacts with growing particle number as the chemical potential is changed. Also the vanishing (close to zero) quark number for a system without chemical potential can be observed (magenta).

A comparison of Figure 2.15 (top) and Figure 2.15 (bottom) shows how the same amount of $\mu$ is able to increase the particle number to larger values in the case of larger $\kappa$, meaning lighter particle mass. This is exactly as expected.

The quark mass susceptibility reacts correspondingly (see Figure 2.15).

The values of $q_{\text{cut}}$ in Figure 2.15 and Figure 2.16 were the same as in Figure 2.13 and will also be taken for the evaluation of the internal energy and the heat capacity.

**Internal Energy and Heat Capacity**

The last two observables which are going to be considered are the internal energy and the heat capacity of the system at finite chemical potential.

The internal energy can be obtained as derivative of the logarithm of the partition function with respect to $\beta$. The fugacity expansion gives the result

$$U = \langle S \rangle = \frac{\sum_q e^{\mu q} \langle \tilde{D}_q \cdot S_\mu \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0}. \quad (2.36)$$

The derivative of the internal energy with respect to $\beta$ gives the heat capacity

$$C = \langle S^2 \rangle - \langle S \rangle^2, \quad (2.37)$$

where we defined

$$\langle S^n \rangle_\mu = \frac{\sum_q e^{\mu q} \langle \tilde{D}_q S^n \rangle_0}{\sum_q e^{\mu q} \langle \tilde{D}_q \rangle_0}. \quad (2.38)$$

The following figures show $U$ and $C$ as function of temperature for two values of $\kappa$ and for chemical potential up to 1.

Figure 2.17 shows that the system lowers its energy when going into the phase with broken symmetry. It can be observed, that the transitions softens with increasing chemical potential. The softened transitions can be seen even better in the heat capacity in Figure 2.18, leading to broader curves. Here also the decrease of the critical temperature with increasing chemical potential can be observed (at $\kappa = 0.01$ the result for $\mu = 1$ has been omitted for earlier mentioned reasons).
2.5. Observables in the Fugacity Expansion

Figure 2.17.: Internal energy as function of temperature at $\kappa = 0.01$ (top) and at $\kappa = 0.001$ (bottom) on a $16^3$ lattice ($10^6$ measurements).
2. Fugacity Expansion

Figure 2.18.: Heat capacity as function of temperature at $\kappa = 0.01$ (top) and at $\kappa = 0.001$ (bottom) on a $16^3$ lattice (10^6 measurements).
2.5. Observables in the Fugacity Expansion

2.5.3. Comparison to Flux Representation Results

After the considerations concerning the dependence of the observables on increasing chemical potential, it must be checked to which extent results obtained in terms of dual variables have been reproduced. To this purpose some direct comparisons are shown. All compared data is obtained from $10^6$ measurements on $16^3$ lattices for values of $q_{cut}$ as in Figure 2.13.

Polyakov Loop

![Polyakov Loop graphs](image)

**Figure 2.19.** Polyakov loop for $\kappa = 0.001$: Comparison to flux representation results.
2. Fugacity Expansion

Figure 2.20.: Polyakov loop for $\kappa = 0.01$: Comparison to flux representation results. All data is obtained from $10^6$ measurements on $16^3$ lattices.

Starting with the Polyakov loop, very good agreement with dual variable results is found for observables obtained with fugacity expansion techniques.
Polyakov Loop Susceptibility

The critical temperature is obtained from the maxima of second derivatives of the logarithm of the partition function. For this reason it is important that also $\chi_P$ is reproduced correctly.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure221.png}
\caption{Polyakov loop susceptibility for $\kappa = 0.001$: Comparison to flux representation results from $10^6$ measurements on $16^3$ lattices.}
\end{figure}
2. Fugacity Expansion

Figure 2.22: Polyakov loop susceptibility for $\kappa = 0.01$: Comparison to flux representation results. All data is obtained from $10^6$ measurements on $16^3$ lattices.

The correspondence found in the comparison of the order parameter is validated in its susceptibility $\chi_P$ for $\kappa = 0.001$, whereas the expected discrepancy for $\kappa = 0.01$ at sufficiently large $\mu$ can be observed.
2.5. Observables in the Fugacity Expansion

Internal Energy

The next observables in consideration are the internal energy and the heat capacity.

Figure 2.23.: Internal energy for $\kappa = 0.001$: Comparison to flux representation results. All data is obtained from $10^6$ measurements on $16^3$ lattices.
Figure 2.24.: Internal energy for $\kappa = 0.01$: Comparison to flux representation results from $10^6$ measurements on $16^3$ lattices.

The results of the internal energy match the outcome of the dual variable technique to a large extent for $\mu \leq 1$. It is also remarkable that $U$ seems to be a quantity that is not as sensitive as the Polyakov loop concerning the expansion technique, since the error is smaller for the data point at $\tau = 0.165$ for $\kappa = 0.01$ for $\mu = 1$. 
2.5. Observables in the Fugacity Expansion

Heat Capacity

Figure 2.25: Heat capacity for $\kappa = 0.001$: Comparison to flux representation results. All compared data is obtained from $10^6$ measurements on $16^3$ lattices for values of $q_{\text{cut}}$ as in Figure 2.13.
2. Fugacity Expansion

Figure 2.26.: Heat capacity for $\kappa = 0.01$: Comparison to flux representation results. All data is obtained from $10^6$ measurements on $16^3$ lattices.

The agreement found for the internal energy is confirmed by Figure 2.26 and Figure 2.25. Also the error in the heat capacity for $\kappa = 0.01$ at $\mu = 1$ is not as big as in the Polyakov loop susceptibility, which was to be expected because of the smaller discrepancy in Figure 2.24.
2.5. Observables in the Fugacity Expansion

**Particle Number**

Since the particle number is very sensitive to changing chemical potential, it is interesting to check for the correctness of the data produced using fugacity expansion.

![Graphs showing particle number for different chemical potentials](image)

**Figure 2.27.** Particle number for $\kappa = 0.001$: Comparison to flux representation results. All data is obtained from $10^6$ measurements on $16^3$ lattices.
The results in terms of fugacity expansion show good agreement to those obtained by flux representation techniques for $\mu \leq 1$. The sensitivity of $q$ seems to be in the same range as that of $P$: $q$ shows only a small mismatch for the known datapoint for the higher value of inverse mass parameter.
2.5. Observables in the Fugacity Expansion

Particle Number Susceptibility

Figure 2.29.: Particle number susceptibility for $\kappa = 0.001$: Comparison to dual variable data. All data is obtained from $10^6$ measurements on $16^3$ lattices.
Figure 2.30.: Particle number susceptibility for $\kappa = 0.01$: Comparison to flux representation results from $10^6$ measurements on $16^3$ lattices.

To summarize the displayed comparison, it can be stated that results obtained in terms of fugacity expansion techniques are in good agreement with the outcome of the flux representation calculation at $\kappa = 0.001$. For higher values of inverse mass parameter (e.g. $\kappa = 0.01$) there seem to be difficulties at $\mu = 1$. In the introduction, we showed the phase diagram according to the center group (Figure 1.1 from [7], where it can be seen that higher values of the chemical potential have to be analyzed. This will be done in Chapter [5]. Moreover, it arises the question, why it is harder to use expansion techniques to bypass the complex action problem for higher values of $\kappa$. Some insight about this matter shall be given in the following section about the
complex action problem and its dependence on chemical potential and inverse mass parameter.
3. Complex Action Problem: Reweighting

It could be seen, that the fugacity expansion is able to reproduce the results achieved in terms of dual variables to a certain extent, concerning the chemical potential in \[2.5.3\]. It is now interesting to investigate at which value of \( \mu \) the complex action problem becomes severe to judge the significance of the obtained outcomes. Furthermore, a dependence on the inverse mass parameter \( \kappa \) is expected from the results displayed in \[2.5.3\].

To this purpose reweighting methods can be used as follows: The partition sum has to be written in a form where one can separate the real and the imaginary part in the exponential function

\[
Z = \sum_{\{P\}} \exp \left( \tau \sum_{x,\nu} \left[ P_x P_{x+\nu} + c.c \right] + 2\kappa \cosh (\mu) \Re(H) + 2i\kappa \sinh (\mu) \Im(H) \right). \tag{3.1}
\]

Subsequently one uses just the real part in the action and puts the imaginary part into a phase.

\[
Z = \sum_{\{P\}} e^{-\tilde{S} + i\phi} = \sum_{\{P\}} e^{-\tilde{S}} e^{i\phi}. \tag{3.2}
\]

\( \tilde{S} \) obviously denotes the real part of the action \[3.1\].

The mean value of an arbitrary observables \( O \) in terms of \( \tilde{S} \) is now given by

\[
\langle O \rangle_{\tilde{S}'} = \frac{\sum_{\{P\}} e^{-\tilde{S}} O e^{i\phi}}{\sum_{\{P\}} e^{-\tilde{S}} e^{i\phi}} = \frac{\langle O e^{i\phi} \rangle_{\tilde{S}'} \langle e^{i\phi} \rangle_{\tilde{S}'}}{\langle e^{i\phi} \rangle_{\tilde{S}'}}. \tag{3.3}
\]

This equation enables the determination of the range of \( \mu \) where the complex action problem becomes severe. As long as the chemical potential is zero, the phase is one and expectation values \[3.3\] are exact. Increasing \( \mu \) leads to uncertainty concerning the contribution of the phase in \[3.3\]. The quantity \( \langle e^{i\phi} \rangle_{\tilde{S}'} \) can therefore be used as a ”measure” of the complex action problem.

The following plots show the dependence of \( \langle e^{i2\phi} \rangle_{\tilde{S}'} \) on the chemical potential for the same four values of \( \kappa \) as in Figure \[1.1\] from \[7\], since these are used for the calculation of observables with expansion techniques and compared to flux representation results in Chapter \[5\].
3. **Complex Action Problem: Reweighting**

![Figure 3.1](image)

**Figure 3.1.** $\langle e^{2i\phi} \rangle_{S'}$ as a function of chemical potential at $\kappa = 0.001$ (a) and $\kappa = 0.01$ (b) for various values of $\tau$ on $16^3$ lattices for $10^5$ measurements.

From the comparison of the data at $\mu = 1$ of Figure 3.1(a) and Figure 3.1(b) it can be understood, why observables for the smaller value of $\kappa$ were more difficult to calculate for smaller temperatures. For example the datapoints in Figure 2.22 show large errorbars for $\tau < 0.175$ which is exactly the temperature range where the complex action problem is prominent (Figure 3.1(b)). In contrast, $\langle e^{2i\phi} \rangle_{S'}$ tends to zero more moderately at $\kappa = 0.001$ for $0.18 \leq \tau \leq 0.183$ in Figure 3.1(a), leading to acceptable results in Figure 2.21.
Due to the fact that there are two more values of $\kappa$ in Figure 1.1 which are going to be used in Chapter 5, also graphs for $\kappa = 0.005$ and $\kappa = 0.1$ are shown in Figure 3.2.

Figure 3.2: $\langle e^{i2\phi} \rangle_{S'}$ as a function of chemical potential for $\kappa = 0.005$ (a) and $\kappa = 0.1$ (b) for various values of $\tau$ on $16^3$ lattices for $10^5$ measurements.

Figure 3.1 - Figure 3.2 show the increasing sensitivity (regarding the chemical potential) of the system concerning the complex action problem for increasing values of $\kappa$. Since $\langle e^{i2\phi} \rangle_{S'}$ tends to zero more rapidly for smaller temperatures and Figure 2.14 (bottom) displayed how increasing the chemical potential leads to smaller values of $\tau_c$, the determination of the critical behaviour for higher values of $\mu$ is additionally com-
3. Complex Action Problem: Reweighting

It can be observed that the range of chemical potential, where fugacity expansion techniques fail to converge, coincides with the region where the complex action problem is dominant.

To which extent these difficulties can be overcome by better statistics will be studied in Chapter 5. Alternatively one could try to bypass the complex action problem via Taylor expansion techniques, this is what will be done in the following chapter.
4. Taylor Expansion Techniques

Another application for the results of the $\mathbb{Z}_3$ Potts model is to compare observables at finite chemical potential from Taylor expansion methods. In this work two kinds of Taylor expansion techniques are studied. The first one, which is going to be investigated, is referred to as "regular Taylor expansion" and discussed in Section 4.4. In this section the logarithm of the partition function itself is Taylor expanded in $\mu$ and derivatives at $\mu = 0$ are the coefficients of the resulting sum. Hereafter, observables can be obtained as derivatives of the expanded logarithm of the partition function at finite chemical potential. The second Taylor expansion method is the so called "improved Taylor expansion" which will be the topic of the second section of this chapter. There we are going to rewrite the exponential function in the partition sum, separating the $\mu$-dependent part. The $\mu$-independent part of the partition function can then be Taylor expanded and further Taylor expansion gives the logarithm of the partition sum. In this way the required logarithm of the partition function can again be used to calculate observables. In both cases the Polyakov loop, particle number and the two corresponding susceptibilities are calculated. After the analysis of the observables at finite chemical potential, the results are compared to those obtained in terms of dual variables for a certain range of $\mu$. The comparison of the two Taylor expansion techniques is conclusively dealt with in Chapter 5.

4.1. Regular Taylor Expansion for the $\mathbb{Z}_3$ Spin Model with Chemical Potential

4.1.1. Partition Function at Finite Chemical Potential in Terms of Regular Taylor Expansion

As already mentioned, the outcome of the $\mathbb{Z}_3$ spin model familiar from Section 2.4 can be used as reference data for the Taylor series. The action is defined as in (2.1)

$$S_{\mu}[P] = -\tau \sum_x \sum_{\nu=1}^3 \left[ P_x \cdot P_{x+\nu}^* + c.c. \right] - \eta \sum_x P_x - \bar{\eta} \sum_x P_x^*$$

(4.1)

and $\eta$ and $\bar{\eta}$ are the quantities introducing the chemical potential as before

$$\eta = \kappa \cdot e^\mu,$$

(4.2)

$$\bar{\eta} = \kappa \cdot e^{-\mu}.$$

(4.3)
4. Taylor Expansion Techniques

The degrees of freedom are the center elements, given by

\[ P_x \in \left\{ 1, e^{\frac{2\pi}{3}}, e^{-\frac{2\pi}{3}} \right\}. \quad (4.4) \]

Also the definition

\[ H = \sum_x P_x, \quad (4.5) \]

will be used again. The partition function reads

\[ Z_{\mu,J} = \sum_{\{P\}} e^{\tau \sum_{x,\nu}\left[ P_x P_{x+\nu}^* \right] + JH + \eta H^* + \bar{\eta} H^*}, \quad (4.6) \]

where \( J \) is a newly introduced source term.

The logarithm of the partition function for \( \mu \neq 0 \) is given via its Taylor expansion and reads

\[ \ln Z_{\mu,J} = \ln Z_{0,J} + \mu \left[ \frac{\partial}{\partial \mu} \ln Z_{\mu,J} \right]_{\mu=0} + \frac{\mu^2}{2} \left[ \frac{\partial^2}{\partial \mu^2} \ln Z_{\mu,J} \right]_{\mu=0} + \frac{\mu^3}{6} \left[ \frac{\partial^3}{\partial \mu^3} \ln Z_{\mu,J} \right]_{\mu=0} + \ldots \quad (4.7) \]

For the calculation of the derivatives with respect to \( \mu \) we use the following abbreviation

\[ D_{\pm} \equiv \eta H \pm \bar{\eta} H^*. \quad (4.8) \]

The derivative of (4.8) with respect to \( \mu \) yields

\[ \frac{\partial}{\partial \mu} D_{\pm} = D_{\mp}. \quad (4.9) \]

The next equations are the computed derivatives, required in (4.7). Starting with the first derivative with respect to \( \mu \), one obtains

\[ \frac{\partial}{\partial \mu} \ln Z_{\mu,J} = \frac{1}{Z_{\mu,J}} \sum_P e^{-S_\mu + JH} \cdot D_- = \langle D_- \rangle_{\mu,J}, \quad (4.10) \]

whereas the second derivative with respect to \( \mu \) yields

\[ \frac{\partial^2}{\partial \mu^2} \ln Z_{\mu,J} = \frac{1}{Z_{\mu,J}} \sum_P e^{-S_\mu + JH} \cdot \left[ D_-^2 + D_+ \right] - \langle D_- \rangle_{\mu,J}^2 \]
\[ = \langle D_- \rangle_{\mu,J} + \langle D_+ \rangle_{\mu,J} - \langle D_- \rangle_{\mu,J}^2. \quad (4.11) \]

One easily finds the following general formula for the derivative with respect to \( \mu \) of the expectation value of an arbitrary operator \( X \)

\[ \frac{\partial}{\partial \mu} \langle X \rangle_{\mu,J} = \langle XD_- \rangle_{\mu,J} + \left\langle \frac{\partial}{\partial \mu} X \right\rangle_{\mu,J} - \langle X \rangle \langle D_- \rangle_{\mu,J}. \quad (4.12) \]
4.1. Regular Taylor Expansion for the $Z_3$ Spin Model with Chemical Potential

(4.12) simplifies the computational effort and the third derivative with respect to $\mu$
reads
\[
\frac{\partial^3}{\partial \mu^3} \ln Z_{\mu,J} = \langle D_3 \rangle_{\mu,J} - 3 \langle D_2 \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} + 2 \langle D_- \rangle^3_{\mu,J} + 3 \langle D_- D_+ \rangle_{\mu,J} - 3 \langle D_+ \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} + \langle D_- \rangle_{\mu,J}.
\] (4.13)

Since we are going to calculate observables up to the third order of $\mu$, also the fourth
derivative of the logarithm of the partition function with respect to $\mu$ has to be calcu-
lated using (4.12).

\[
\frac{\partial^4}{\partial \mu^4} \ln Z_{\mu,J} = \langle D_4 \rangle_{\mu,J} - 6 \langle D_- \rangle^4_{\mu,J} + 6 \langle D_2 D_+ \rangle_{\mu,J} - 4 \langle D_2 \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} - 12 \langle D_- D_+ \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} + 12 \langle D_2 \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} - 3 \langle D_2 \rangle_{\mu,J} - 3 \langle D_- \rangle_{\mu,J} \langle D_+ \rangle_{\mu,J} - 12 \langle D_- \rangle^2_{\mu,J} \langle D_+ \rangle_{\mu,J}.
\] (4.14)

Inserting the results (4.10) - (4.14) in (4.7) gives the required expansion of the logarithm
of the partition function for finite chemical potential
\[
\ln Z_{\mu,J} = \ln Z_{0,J} + \mu \langle D_- \rangle_{0,J} + \frac{\mu^2}{2} \left[ \langle D_2 \rangle_{0,J} + \langle D_+ \rangle_{0,J} - \langle D_- \rangle_{0,J} \right] + \frac{\mu^3}{6} \left[ \langle D_3 \rangle_{0,J} - 3 \langle D_2 \rangle_{0,J} \langle D_- \rangle_{0,J} + 2 \langle D_- \rangle^3_{0,J} + 3 \langle D_- D_+ \rangle_{0,J} - 3 \langle D_+ \rangle_{0,J} \langle D_- \rangle_{0,J} + \langle D_- \rangle_{0,J} \right]
+ \frac{\mu^4}{24} \left[ \langle D_4 \rangle_{\mu,J} - 6 \langle D_- \rangle^4_{\mu,J} + 6 \langle D_2 D_+ \rangle_{\mu,J} - 4 \langle D_2 \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} - 12 \langle D_- D_+ \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} + 12 \langle D_2 \rangle_{\mu,J} \langle D_- \rangle_{\mu,J} + 3 \langle D_2 \rangle_{\mu,J} + 3 \langle D_- \rangle_{\mu,J} \langle D_+ \rangle_{\mu,J} - 4 \langle D_- \rangle_{\mu,J} - 3 \langle D_+ \rangle_{\mu,J} + 12 \langle D_- \rangle_{\mu,J} \langle D_+ \rangle_{\mu,J} \right].
\] (4.15)
4. Taylor Expansion Techniques

4.1.2. Calculation of Observables in Terms of Regular Taylor Expansion

As the logarithm of the partition function for finite chemical potential was obtained using Taylor expansion (4.15), we are now able to calculate observables and start with the particle number of the system and its susceptibility.

Particle Number and Particle Number Susceptibility

The particle number has been defined in (2.13) as first derivative of the logarithm of the partition function with respect to chemical potential. Using Taylor expansion (4.15), we are now able to calculate observables and start with

4.1.2. Calculation of Observables in Terms of Regular Taylor Expansion

\[ \langle q \rangle_\mu = \frac{\partial}{\partial \mu} \ln Z_{\mu,0} = \langle D_- \rangle_{0,0} \]

\[ + \mu \left[ \langle D_-^2 \rangle_{0,0} + \langle D_+ \rangle_{0,0} - \langle D_- \rangle_{0,0}^2 \right] \]

\[ + \frac{\mu^2}{2} \left[ \langle D_-^3 \rangle_{0,0} - 3 \langle D_- \rangle_{0,0} \langle D_- \rangle_{0,0}^2 + 2 \langle D_- \rangle_{0,0}^3 \right] \]

\[ + 3 \langle D_- \rangle_{0,0} \langle D_+ \rangle_{0,0} - 3 \langle D_+ \rangle_{0,0} \langle D_- \rangle_{0,0} + \langle D_+ \rangle_{0,0} \]

\[ + \frac{\mu^3}{6} \left[ \langle D_-^4 \rangle_{0,0} - 6 \langle D_- \rangle_{0,0}^4 + 6 \langle D_-^2 D_+ \rangle_{0,0} \right] \]

\[ - 4 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} - 12 \langle D_- D_+ \rangle_{0,0} \langle D_- \rangle_{0,0} \]

\[ + 12 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} - 3 \langle D_- \rangle_{0,0}^2 - 6 \langle D_+ \rangle_{0,0}^2 \]

\[ + 3 \langle D_- \rangle_{0,0}^3 + 3 \langle D_+ \rangle_{0,0}^2 - 4 \langle D_- \rangle_{0,0} \]

\[ - 3 \langle D_+ \rangle_{0,0}^2 + \langle D_- \rangle_{0,0}^4 + \langle D_+ \rangle_{0,0} + 12 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} \]

\[ + O(\mu^4) \]  

Since the particle number susceptibility is the derivative of \( \langle q \rangle_\mu \) with respect to \( \mu \) (2.15), one finds

\[ \chi_{q\mu} = \frac{\partial^2}{\partial \mu^2} \ln Z_{\mu,0} = \left[ \langle D_-^2 \rangle_{0,0} + \langle D_+ \rangle_{0,0} - \langle D_- \rangle_{0,0}^2 \right] \]

\[ + \mu \left[ \langle D_-^3 \rangle_{0,0} - 3 \langle D_- \rangle_{0,0} \langle D_- \rangle_{0,0}^2 + 2 \langle D_- \rangle_{0,0}^3 \right] \]

\[ + 3 \langle D_- \rangle_{0,0} \langle D_+ \rangle_{0,0} - 3 \langle D_+ \rangle_{0,0} \langle D_- \rangle_{0,0} + \langle D_+ \rangle_{0,0} \]

\[ + \frac{\mu^2}{2} \left[ \langle D_-^4 \rangle_{0,0} - 6 \langle D_- \rangle_{0,0}^4 + 6 \langle D_-^2 D_+ \rangle_{0,0} \right] \]

\[ - 4 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} - 12 \langle D_- D_+ \rangle_{0,0} \langle D_- \rangle_{0,0} \]

\[ + 12 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} - 3 \langle D_- \rangle_{0,0}^2 - 6 \langle D_+ \rangle_{0,0}^2 \]

\[ + 3 \langle D_- \rangle_{0,0}^3 + 3 \langle D_+ \rangle_{0,0}^2 - 4 \langle D_- \rangle_{0,0} \]

\[ - 3 \langle D_+ \rangle_{0,0}^2 + \langle D_- \rangle_{0,0}^4 + \langle D_+ \rangle_{0,0} + 12 \langle D_- \rangle_{0,0}^2 \langle D_+ \rangle_{0,0} \]
The expectation value of the Polyakov loop for finite chemical potential is given by

\[ \langle P \rangle_{\mu} = \frac{\partial}{\partial J} \ln Z_{\mu,J} \bigg|_{J=0}. \]  

(4.17)

The next observables we consider are the Polyakov loop and its susceptibility.

**Polyakov Loop**

The expectation value of the Polyakov loop for finite chemical potential is given by

\[ \langle P \rangle_{\mu} = \frac{\partial}{\partial J} \ln Z_{\mu,J} \bigg|_{J=0}. \]  

(4.18)

The calculation of (4.18) requires the derivative with respect to \( J \) for an arbitrary observable \( X \) which is given by

\[ \frac{\partial}{\partial J} \langle X \rangle_{0,J} = \frac{\partial}{\partial J} \frac{1}{Z_{0,J}} \sum_{\{P\}} e^{-S_0 + JH} X, \]  

(4.19)

and hence the simplifying equation

\[ \frac{\partial}{\partial J} \langle X \rangle_{0,J} = \langle XH \rangle_{0,0} - \langle X \rangle_{0,J} \langle H \rangle_{0,J}, \]  

(4.20)

can be found. The use of (4.20) makes the computation of (4.18) easier and yields

\[ \langle P \rangle_{\mu} = \langle H \rangle_{0,0} \]

\[ + \mu \left[ \langle D_- H \rangle_{0,0} - \langle D_- \rangle_{0,0} \langle H \rangle_{0,0} \right] \]

\[ + \frac{\mu^2}{2} \left[ \langle D^2 H \rangle_{0,0} - \langle D^2 \rangle_{0,0} \langle H \rangle_{0,0} - 2 \langle D_- H \rangle_{0,0} \langle D_- \rangle_{0,0} \right] \]

\[ + \frac{\mu^3}{6} \left[ \langle D^3 H \rangle_{0,0} - \langle D^3 \rangle_{0,0} \langle H \rangle_{0,0} - 3 \langle D^2 H \rangle_{0,0} \langle D_- \rangle_{0,0} + 6 \langle D^2 \rangle_{0,0} \langle D_- \rangle_{0,0} \langle H \rangle_{0,0} \right] \]

\[ - 3 \langle D_-^2 \rangle_{0,0} \langle D_- H \rangle_{0,0} + 6 \langle D_- H \rangle_{0,0} \langle D_- \rangle_{0,0}^2 - 6 \langle D_- \rangle_{0,0}^3 \langle H \rangle_{0,0} \]

\[ + 3 \langle D_- D_+ H \rangle_{0,0} - 3 \langle D_- D_+ \rangle_{0,0} \langle H \rangle_{0,0} - 3 \langle D_- H \rangle_{0,0} \langle D_+ \rangle_{0,0} - 3 \langle D_+ H \rangle_{0,0} \langle D_- \rangle_{0,0} \]

\[ + 6 \langle D_- \rangle_{0,0} \langle D_+ \rangle_{0,0} \langle H \rangle_{0,0} + \langle D_- \rangle_{0,0} \langle D_- H \rangle_{0,0} - \langle D_- \rangle_{0,0} \langle H \rangle_{0,0} \rangle \]

\[ + O (\mu^4). \]  

(4.21)
4. Taylor Expansion Techniques

Polyakov Loop Susceptibility

In the same way as (4.21) was obtained, also the Polyakov loop susceptibility can be calculated using (4.18) and (4.7)

\[ \chi_P = \frac{\partial^2}{\partial J^2} \ln Z_{\mu,J} \bigg|_{\mu=0} = \langle H^2 \rangle_{0,0} - \langle H \rangle_{0,0}^2 + \mu \left[ \langle D_- H^2 \rangle_{0,0} - 2 \langle D_- H \rangle_{0,0} \langle H \rangle_{0,0} + 2 \langle D_- \rangle_{0,0} \langle H \rangle_{0,0}^2 - \langle D_- \rangle_{0,0} \langle H^2 \rangle_{0,0} \right] \]

\[ + \frac{\mu^2}{2} \left[ \langle D_-^2 H^2 \rangle_{0,0} - 4 \langle D_-^2 H \rangle_{0,0} \langle H \rangle_{0,0} + \langle D_-^2 \rangle_{0,0} \langle H^2 \rangle_{0,0} + \langle D_-^2 \rangle_{0,0} \langle H \rangle_{0,0}^2 - \langle D_- \rangle_{0,0} \langle H^2 \rangle_{0,0} \right] \]

\[ + \frac{\mu}{2} \left[ \langle D_+ H \rangle_{0,0} - \langle D_+ \rangle_{0,0} \langle H \rangle_{0,0}^2 + 2 \langle D_+ \rangle_{0,0} \langle H \rangle_{0,0}^2 \right] + O(\mu^3). \]

(4.22)

4.1.3. Analysis of Observables in Terms of Regular Taylor Expansion

The analysis of the observables obtained in terms of regular Taylor expansion will be carried out as follows. Firstly, we compare the outcome of (4.16), (4.17), (4.21) and (4.22) to dual variable data for the same values of \( \kappa \) and some values of chemical potential as in 2.5.3, where a look at the composition of the orders in the regular Taylor expansion is taken. Secondly, the coefficients of the Polyakov loop and the corresponding susceptibility in the regular Taylor series will be shown to study convergence properties.

Comparison to Dual Variable Data

For the comparison of the regular Taylor series methods (RTE) to the fugacity expansion technique, the same statistics as in 2.5.3 is used. This means all data points are for \( 10^6 \) measurements on \( 16^3 \) lattices in the following section. Moreover, the same values of \( \kappa \) are analyzed.

The final comparison of all three series expansions of this work, also for other values of \( \kappa \) and chemical potential, is conclusively dealt with in Chapter 5.

The following figures show how the orders of the regular Taylor series add up to approach the flux representation results. The label RTE \( O(\mu^3) \) stands for the result of the sum up to third order of \( \mu \): \( O(\mu^0) + O(\mu^1) + O(\mu^2) + O(\mu^3) \), for example. First derivatives of the logarithm of the partition function (Polyakov loop and particle number) are computed and shown for third order of \( \mu \) and derivatives of second order of (4.15) are shown for \( \mu \) up to second order (Polyakov loop susceptibility and particle
4.1. Regular Taylor Expansion for the \( \mathbb{Z}_3 \) Spin Model with Chemical Potential

Following the conventions of 2.5.3, we begin our analysis with the comparison of the Polyakov loop \( (4.21) \) to the outcome of dual variable data for \( \kappa = 0.001 \).

![Figure 4.1](image)

**Figure 4.1.** Polyakov loop obtained in terms of regular Taylor expansion for \( \kappa = 0.001 \) as function of temperature. Shown are results up to third order in \( \mu \) (RTE \( O(\mu^3) \), green) which are compared to flux representation results (red).

Although the Polyakov loop for \( \kappa = 0.001 \) can be computed using regular Taylor series expansion up to third order of \( \mu \) for finite chemical potential, Figure 4.1 shows that already for \( \mu = 0.8 \) discrepancies to flux representation results arise. For this relatively small value of \( \kappa \), the region where the complex action problem is severe is not reached, as shown in Figure 3.1(a). It can also be seen, that an additional order does not necessarily mean an immediate improvement for all values of \( \tau \) in the outcome (RTE \( O(\mu^0) \) and RTE \( O(\mu^1) \)). However, the results for the Polyakov loop up to third order of \( \mu \) are quite accurate, since they are used to calculate the corresponding susceptibility which shows convergence to dual variable data when the third order of \( \mu \) is included, see Figure 4.3. The coefficients that lead to this outcome are shown in

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The next value of $\kappa$ for which the Polyakov loop is analyzed is $\kappa = 0.01$, familiar from 2.5.3. From this section it could be expected, that the discrepancies increase with increasing $\kappa$, meaning decreasing particle mass.

However, the results for the Polyakov loop in Figure 4.2 seem to have similar agreements with the outcome obtained in terms of the flux representation below $\mu = 0.8$ and likewise discrepancies above this value of chemical potential. Nevertheless, the increasing difficulties calculating observables for higher values of $\kappa$, e.g. $\kappa = 0.01$ surface in the second derivative of the logarithm of the partition function with respect to $J$ shown in Figure 4.3 and Figure 4.4.

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Figure 4.9

The next value of $\kappa$ for which the Polyakov loop is analyzed is $\kappa = 0.01$, familiar from 2.5.3. From this section it could be expected, that the discrepancies increase with increasing $\kappa$, meaning decreasing particle mass.
Figure 4.3.: Polyakov loop susceptibility obtained in terms of regular Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to third order in $\mu$ (RTE $O(\mu^3)$, green) which are compared to flux representation results (red).

From Figure 4.3 it can be seen, that the additional third order of $\mu$ improves convergence for small values of chemical potential ($\mu < 0.8$). For $\mu > 0.8$ results in terms of regular Taylor expansion fail to reproduce dual variable data. This breakdown is even more prominent in Figure 4.4 which shows the Polyakov loop susceptibility for $\kappa = 0.01$. 

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Figure 4.4.: Polyakov loop susceptibility obtained in terms of regular Taylor expansion for $\kappa = 0.01$ as function of temperature. Shown are results up to third order in $\mu$ (RTE $\mathcal{O}(\mu^3)$, green) which are compared to flux representation results (red).

Figure 4.4 shows that also the regular Taylor expansion seems to be sensitive to the region of chemical potential where the complex phase problem is dominant. For $\kappa = 0.01$ and the temperatures used in Figure 4.4 this is near values of $\mu = 1$ (see Chapter 3). The comparison of Figure 4.3 and Figure 4.4 confirms this, since it could be expected that the Polyakov loop susceptibility would be more difficult to calculate for higher values of $\kappa$.

From Figure 4.4 it can be seen, that a reliable calculation of $\chi_P$ for $\kappa = 0.01$ is only possible for very small values of chemical potential. Great differences of the dual variable data and the results obtained in terms of regular Taylor expansion arise at $\mu = 0.6$ already. Since the critical temperature can be found via second derivatives of the logarithm of the partition function, for example $\chi_P$, only a small region of the phase diagram of the effective center model (shown in 7) can be expected to be analyzable in terms of regular Taylor expansion including the third order of $\mu$. 

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4.1. Regular Taylor Expansion for the $\mathbb{Z}_3$ Spin Model with Chemical Potential

The next observables which are going to be analyzed are the particle number for $\kappa = 0.001$ (Figure 4.5) and $\kappa = 0.01$ (Figure 4.6). Results up to third order of $\mu$ are shown.

Figure 4.5.: Particle number obtained in terms of regular Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to third order in $\mu$ (RTE $O(\mu^3)$, green) which are compared to flux representation results (red).

Since the particle number is obtained as derivative of (4.15) with respect to $\mu$, one loses an order of $\mu$ in the calculation. Moreover, as can be seen from Figure 4.5 and Figure 4.6, only odd orders of $\mu$ contribute to the regular Taylor expansion series. RTE $O(\mu)$ and RTE $O(\mu^2)$ are congruent. This means that the particle number is more cumbersome to calculate.

Nevertheless, the observation of $q$ can serve as consistency check of (4.15) and displays also the difficulties of the regular Taylor series arising already at $\mu = 0.8$. The same behaviour can be observed in the following graph for $\kappa = 0.01$ (Figure 4.6).
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Figure 4.6.: Particle number obtained in terms of regular Taylor expansion for $\kappa = 0.01$ as function of temperature. Shown are results up to third order in $\mu$ (RTE $O(\mu^3)$, green) which are compared to flux representation results (red).
4.1. Regular Taylor Expansion for the $\mathbb{Z}_3$ Spin Model with Chemical Potential

The following Figures show the particle number susceptibility (4.17) for $\kappa = 0.001$ (Figure 4.7) and $\kappa = 0.01$ (Figure 4.8), evaluated up to second order of chemical potential.

**Figure 4.7.:** Particle number obtained in terms of regular Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to third order in $\mu$ (RTE $O(\mu^3)$, green) which are compared to flux representation results (red).

As expected from the observation of the Polyakov loop susceptibility (Figure 4.3, Figure 4.4), the second order derivative of the logarithm of the partition function with respect to $\mu$ (4.17) shows discrepancies to results obtained in terms of dual variables, even for small values of $\mu$ (Figure 4.7). This means that also the particle number susceptibility obtained in terms of regular Taylor expansion up to second order in $\mu$ can only be used to analyze the phase diagram of the effective center model (shown in [7]) to small extent.

Also for higher values of $\kappa$, no improvement concerning the convergence of the regular Taylor series can be observed (see Figure 4.8).
To summarize the above comparison of results obtained in terms of regular Taylor expansion to the outcome of flux representation techniques, it can be said that the observables can only be calculated for small values of chemical potential using (4.16), (4.17), (4.21) and (4.22). It should also be mentioned, that the fugacity expansion technique showed good agreement in a larger range of chemical potential for the same values of $\kappa$ and $\mu$ and the same statistics (2.5.3).

The reason for the discrepancies in the calculated observables may be found by observing the coefficients of the regular Taylor series. This will be done in the following.
4.1. Regular Taylor Expansion for the $\mathbb{Z}_3$ Spin Model with Chemical Potential

Analysis of the Coefficients in the Regular Taylor Series

The observables in terms of the regular Taylor series are computed in the following way:

$$O(\mu) = \sum_{i=0}^{N} \mu^i \cdot c_i,$$

where $O$ denotes an arbitrary observable. The coefficients $c_i$ are shown for the Polyakov loop and the Polyakov loop susceptibility for $N = 3$ in Figure 4.9.

![Coefficient plots](image)

**Figure 4.9.** Coefficients of the regular Taylor expansion for the Polyakov loop (top) and the Polyakov loop susceptibility (bottom) for $\kappa = 0.001$ (left) and $\kappa = 0.01$ (right) as function of temperature. The coefficients are shown up to third order in $\mu$ (RTE coeff $O(\mu^3)$, red).

In Figure 4.9 it can be seen, that especially for $\chi_P$ the coefficients of higher orders of $\mu$ start to show more minima and maxima and also larger error bars. These fluctuations and the error bars in the coefficients of higher orders of $\mu$ are multiplied by powers of $\mu$ when observables are computed. This means that for $\mu > 1$ even higher discrepancies in the evaluation of observables in terms of regular Taylor expansion are to be expected Chapter 5. To which extent the so called improved Taylor expansion is able to reproduce dual variable data will be analyzed in the following section.
4. Taylor Expansion Techniques

4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

Another way of obtaining the logarithm of the partition function for finite chemical potential using Taylor expansion is going to be performed in the next section as follows. Firstly, the action will be reorganized separating the $\mu$-dependent part in the exponential function of the partition sum. This $\mu$-dependent part will be Taylor expanded afterwards, leaving the partition function dependent on $\mu$. The logarithm of the partition function is then obtained using further Taylor expansion.

4.2.1. Partition Sum for $\mu \neq 0$

The starting point of this section is again the familiar effective action \( S_\mu[\{P\}] = -\tau \sum_x \sum_{\nu=1}^3 [P_x \cdot P^*_x + \text{c.c.}] - \eta \sum_x P_x - \bar{\eta} \sum_x P^*_x, \)
where $\eta = \kappa \cdot e^\mu$ and $\bar{\eta} = \kappa \cdot e^{-\mu}$ were already introduced. The degrees of freedom are given by the $\mathbb{Z}_3$ elements

\( P_x \in \{1, e^{\frac{2\pi i}{3}}, e^{-\frac{2\pi i}{3}}\}, \)

and also the abbreviation $H$ is used again and defined as $H = \sum_x P_x$.

Since the action of the model in consideration is known, the partition function can be written as

\[ Z_{\mu,J} = \sum_{\{P\}} e^{-S_{\mu}[\{P\}] + JH}, \]  

(4.24)

where $J$ is a source term. The first step of the improved Taylor expansion is the reorganization of the partition function with the purpose of separating the $\mu$ dependent part of the action from the remainder, which apparently does not depend on the chemical potential. With this in mind, we obtain

\[ Z_{\mu,J} = \sum_{\{P\}} e^{\tau \sum_{x,\nu} [P_x \cdot P^*_x + \text{c.c.}] + JH + \eta H + \bar{\eta} H^*}. \]  

(4.25)

The part of the action with does not depend on $\mu$ (denoted $S_0[\{P\}]$) can now be separated from the rest of the action as follows

\[ Z_{\mu,J} = \sum_{\{P\}} e^{\tau \sum_{x,\nu} [P_x \cdot P^*_x + \text{c.c.}] + JH + \eta H + \bar{\eta} H^*} \]

\[ = \sum_{\{P\}} e^{S_0[\{P\}] + JH + (\eta - \kappa)H + (\bar{\eta} - \kappa)H^*} \]

\[ = \sum_{\{P\}} e^{S_0[\{P\}] + JH + \rho H + \bar{\rho} H^*}. \]  

(4.26)
4.2. Improved Taylor Expansion for the $Z_3$ Spin Model at Finite Chemical Potential

As already mentioned, the part of the exponential function which depends on $\mu$ is intended to be Taylor expanded in $\rho$ and $\bar{\rho}$ which we define as $\rho = \kappa (e^\mu - 1)$ and $\bar{\rho} = \kappa (e^{-\mu} - 1)$. For this purpose, we use the abbreviation

$$R \equiv \rho H + \bar{\rho} H^*,$$

and the Taylor expanded partition function reads:

$$Z_{\mu,J} = \sum_{\{P\}} e^{S_0[P]+JH} \left[ 1 + R + \frac{R^2}{2} + \frac{R^3}{3!} + \frac{R^4}{4!} + \mathcal{O}(\rho^5) \right]$$

$$= Z_{0,J} \left[ 1 + \langle R \rangle + \frac{1}{2} \langle R^2 \rangle + \frac{1}{3!} \langle R^3 \rangle + \frac{1}{4!} \langle R^5 \rangle + \mathcal{O}(\rho^5) \right].$$

(4.28)

However, the calculation of observables requires the logarithm of $Z$. To this end, the Taylor expansion formula for the natural logarithm

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \cdots$$

(4.29)

can be used and the logarithm of the partition function, dependent on $\mu$ can thus be identified in terms of the improved Taylor expansion technique as

$$\ln Z_{\mu,J} = \ln Z_{0,J} + \ln \left[ 1 + \langle R \rangle_{0,J} + \frac{1}{2} \langle R^2 \rangle_{0,J} + \frac{1}{3!} \langle R^3 \rangle_{0,J} + \frac{1}{4!} \langle R^5 \rangle_{0,J} + \mathcal{O}(\rho^5) \right]$$

$$= \ln Z_{0,J} + \langle R \rangle_{0,J} + \frac{1}{2} \langle R^2 \rangle_{0,J} + \frac{1}{3!} \langle R^3 \rangle_{0,J} + \frac{1}{4!} \langle R^5 \rangle_{0,J}$$

$$- \frac{1}{2} \left[ \langle R \rangle_{0,J} + \frac{1}{2} \langle R^2 \rangle_{0,J} + \frac{1}{3!} \langle R^3 \rangle_{0,J} \right]^2$$

$$- \frac{1}{3} \left[ \langle R \rangle_{0,J} + \frac{1}{2} \langle R^2 \rangle_{0,J} \right]^3$$

$$- \frac{1}{4} \langle R \rangle_{0,J}^4$$

$$+ \mathcal{O}(\rho^5).$$

(4.30)

Since it simplifies the subsequent calculations, (4.30) is organized concerning the orders of $R$ (and therefore $\rho$) and yields

$$\ln Z_{\mu,J} = \ln Z_{0,J} + \langle R \rangle_{0,J}$$

$$+ \frac{1}{2} \left[ \langle R^2 \rangle_{0,J} - \langle R \rangle_{0,J}^2 \right]$$

$$+ \frac{1}{6} \left[ \langle R^3 \rangle_{0,J} - 3 \langle R \rangle_{0,J} \langle R^2 \rangle_{0,J} + 2 \langle R \rangle_{0,J}^3 \right]$$

$$+ \frac{1}{24} \left[ \langle R^4 \rangle_{0,J} - 4 \langle R \rangle_{0,J} \langle R^3 \rangle_{0,J} + 12 \langle R \rangle_{0,J}^2 \langle R^2 \rangle_{0,J} - 3 \langle R^2 \rangle_{0,J}^2 - 6 \langle R \rangle_{0,J}^4 \right]$$

$$+ \mathcal{O}(\rho^5).$$

(4.31)
Equation (4.31) allows for the evaluation of observables in terms of the improved Taylor expansion. The particle number \( q \) and its susceptibility \( \chi_q \) are going to be calculated first.

### 4.2.2. Calculation of Observables in Terms of Improved Taylor Expansion

#### Quark Number

The evaluation of the particle number requires derivatives with respect to \( \mu \). For example

\[
\frac{\partial \rho}{\partial \mu} = \frac{\partial}{\partial \mu} \kappa \cdot (e^\mu - 1) = \kappa \cdot e^\mu = \eta, \tag{4.32}
\]

and

\[
\frac{\partial \bar{\rho}}{\partial \mu} = \frac{\partial}{\partial \mu} \kappa \cdot (e^{-\mu} - 1) = -\kappa \cdot e^\mu = -\bar{\eta}. \tag{4.33}
\]

The derivatives of \( \eta \) and \( \bar{\eta} \) with respect to \( \mu \) are given by

\[
\frac{\partial \eta}{\partial \mu} = \eta, \tag{4.34}
\]

and

\[
\frac{\partial \bar{\eta}}{\partial \mu} = -\bar{\eta}. \tag{4.35}
\]

Equation (4.31) shows that also the derivative of \( R \) will be needed for the computation of the particle number. Thus

\[
\frac{\partial}{\partial \mu} R = \frac{\partial}{\partial \mu} (\rho H + \bar{\rho} H^*) = \eta H - \bar{\eta} H^* \equiv D_- \tag{4.36}
\]

Here, the quantity \( D_- \) has been defined. Consequently, the derivative of \( D_- \) with respect to \( \mu \) will also be needed. It gives

\[
\frac{\partial}{\partial \mu} D_- = \frac{\partial}{\partial \mu} (\eta H - \bar{\eta} H^*) = \eta H + \bar{\eta} H^* \equiv D_+, \tag{4.37}
\]

defining \( D_+ \). Finally

\[
\frac{\partial}{\partial \mu} D_+ = \frac{\partial}{\partial \mu} (\eta H + \bar{\eta} H^*) = \eta H - \bar{\eta} H^* \equiv D_- \tag{4.38}
\]
4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

Applying (4.32) - (4.38), the particle number $q$ in terms of the improved Taylor expansion up to the fourth order of $\mu$ is given by

$$
\langle q \rangle_{\mu} = \frac{\partial}{\partial \mu} \ln Z_{\mu,0} = \langle D_- \rangle_{0,0} \\
+ \frac{1}{2} \left[ 2 \langle RD_- \rangle_{0,0} - 2 \langle R \rangle_{0,0} \langle D_- \rangle_{0,0} \right] \\
+ \frac{1}{6} \left[ 3 \langle R^2 D_- \rangle_{0,0} - 3 \langle D_- \rangle_{0,0} \langle R^2 \rangle_{0,0} \\
- 6 \langle R \rangle_{0,0} \langle RD_- \rangle_{0,0} + 6 \langle R \rangle_{0,0}^2 \langle D_- \rangle_{0,0} \right] \\
+ \frac{1}{24} \left[ 4 \langle R^3 D_- \rangle_{0,0} - 4 \langle D_- \rangle_{0,0} \langle R^3 \rangle_{0,0} - 12 \langle R \rangle_{0,0} \langle R^2 D_- \rangle_{0,0} \\
+ 24 \langle R \rangle_{0,0} \langle D_- \rangle_{0,0} \langle R^2 \rangle_{0,0} + 24 \langle R \rangle_{0,0}^2 \langle RD_- \rangle_{0,0} \\
- 12 \langle R \rangle_{0,0} \langle RD_- \rangle_{0,0} - 24 \langle R \rangle_{0,0}^3 \langle D_- \rangle_{0,0} \right] \\
+ \mathcal{O} (\rho^5) .
$$

Equation (4.39) can be organized according to the powers of $R$ as follows:

$$
\langle q \rangle_{\mu} = \langle D_- \rangle_{0,0} \\
+ \langle RD_- \rangle_{0,0} - \langle R \rangle_{0,0} \langle D_- \rangle_{0,0} \\
+ \frac{1}{2} \langle R^2 D_- \rangle_{0,0} - \frac{1}{2} \langle D_- \rangle_{0,0} \langle R^2 \rangle_{0,0} \\
- \langle R \rangle_{0,0} \langle RD_- \rangle_{0,0} + \langle R \rangle_{0,0}^2 \langle D_- \rangle_{0,0} \\
+ \frac{1}{6} \langle R^3 D_- \rangle_{0,0} - \frac{1}{6} \langle D_- \rangle_{0,0} \langle R^3 \rangle_{0,0} - \frac{1}{2} \langle R \rangle_{0,0} \langle R^2 D_- \rangle_{0,0} \\
+ \langle R \rangle_{0,0} \langle D_- \rangle_{0,0} \langle R^2 \rangle_{0,0} + \langle R \rangle_{0,0}^2 \langle RD_- \rangle_{0,0} \\
- \frac{1}{2} \langle R \rangle_{0,0}^3 \langle D_- \rangle_{0,0} - \langle R \rangle_{0,0}^3 \langle D_- \rangle_{0,0} \\
+ \mathcal{O} (\rho^5) .
$$

The particle number susceptibility can be obtained as derivative of (4.40) with respect to $\mu$. 

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**Quark Number Susceptibility**

The particle number susceptibility in terms of the improved Taylor expansion technique up to the fourth order of $\rho$ can also be calculated from (4.31) using (4.32) - (4.38) and is given by

\[
\chi_q(\mu) = \frac{\partial^2}{\partial \mu^2} \ln Z_{\mu,0} \bigg|_{\mu=0} \\
= (D_{+})_{0,0} \\
+ \langle D_{-}\rangle_{0,0} + \langle RD_{+}\rangle_{0,0} - \langle D_{-}\rangle_{0,0}^2 - \langle R\rangle_{0,0} \langle D_{+}\rangle_{0,0} \\
+ \langle RD_{+}\rangle_{0,0} + \frac{1}{2} \langle R^2 D_{+}\rangle_{0,0} - \frac{1}{2} \langle D_{+}\rangle_{0,0} \langle R^2\rangle_{0,0} - \langle D_{-}\rangle_{0,0} \langle RD_{-}\rangle_{0,0} \\
- \langle D_{-}\rangle_{0,0} \langle RD_{-}\rangle_{0,0} - \langle R\rangle_{0,0} \langle D_{-}\rangle_{0,0}^2 - \langle R\rangle_{0,0} \langle D_{+}\rangle_{0,0} \\
+ 2 \langle R\rangle_{0,0} (D_{-})_{0,0}^2 + \langle R\rangle_{0,0}^2 (D_{+})_{0,0} \\
+ \frac{1}{2} \langle R^2 D_{-}\rangle_{0,0} + \frac{1}{2} \langle R^2 D_{+}\rangle_{0,0} + \langle R\rangle_{0,0} \langle R^2\rangle_{0,0} - \frac{1}{2} \langle R\rangle_{0,0} \langle R^2 D_{-}\rangle_{0,0} \\
\sum_{\langle R\rangle_{0,0}^2} \langle R^2 D_{-}\rangle_{0,0} - \langle R\rangle_{0,0} \langle R^2 D_{-}\rangle_{0,0} - \frac{1}{2} \langle R\rangle_{0,0} \langle R^2 D_{-}\rangle_{0,0} \\
+ 2 \langle R\rangle_{0,0} (D_{-})_{0,0}^2 + \langle R\rangle_{0,0}^2 (D_{+})_{0,0} \\
+ \langle R\rangle_{0,0} \langle R^2\rangle_{0,0} - \langle R\rangle_{0,0} \langle RD_{-}\rangle_{0,0} \\
- 3 \langle R\rangle_{0,0}^2 (D_{-})_{0,0} + \langle R\rangle_{0,0} \langle R^2\rangle_{0,0} - \frac{1}{2} \langle R^2 D_{-}\rangle_{0,0} \\
+ O(\rho^3).
\]

(4.41)

**Polyakov Loop**

Since the results of the improved Taylor expansion should be compared to those of the regular Taylor expansion for several observables, there are two more observables to calculate, namely the Polyakov loop and its susceptibility. The expectation value of the Polyakov loop at finite chemical potential is given by

\[
\langle H \rangle_{\mu} = \frac{\partial}{\partial J} \ln Z_{\mu,J} \bigg|_{J=0}.
\]

The derivative of the expectation value of an arbitrary operator $X$ with respect to $J$ is

\[
\frac{\partial}{\partial J} \langle X \rangle_{0,J} = \frac{1}{Z_{0,J}} \sum_{\{P\}} e^{-S_0 + JH} X,
\]

(4.42)

which yields

\[
\frac{\partial}{\partial J} \langle X \rangle_{0,J} = \langle XH \rangle_{0,J} - \langle X \rangle_{0,J} \langle H \rangle_{0,J}.
\]

(4.43)
4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

Therefore, the expectation value of the Polyakov loop at finite chemical potential can be calculated from (4.31) using (4.43) and gives

$$
\langle H \rangle_{\mu} = \langle H \rangle_{0,0} 
+ \langle RH \rangle_{0,0} - \langle R \rangle_{0,0} \langle H \rangle_{0,0}
+ \frac{1}{2} \langle R^2 H \rangle_{0,0} - \frac{1}{2} \langle R^2 \rangle_{0,0} \langle H \rangle_{0,0} - \langle R \rangle_{0,0} \left( \langle RH \rangle_{0,0} - \langle R \rangle_{0,0} \langle H \rangle_{0,0} \right)
+ \frac{1}{6} \langle R^3 H \rangle_{0,0} - \frac{1}{6} \langle R^3 \rangle_{0,0} \langle H \rangle_{0,0} - \frac{1}{2} \langle RH \rangle_{0,0} \langle R^2 \rangle_{0,0} + \langle R \rangle_{0,0} \langle H \rangle_{0,0} \langle R^2 \rangle_{0,0}
- \frac{1}{2} \langle R \rangle_{0,0} \langle R^2 \rangle_{0,0} + \langle R \rangle_{0,0} \langle RH \rangle_{0,0} - \langle R \rangle_{0,0} \langle H \rangle_{0,0}
+ \frac{1}{24} \langle R^4 H \rangle_{0,0} - \frac{1}{24} \langle R^4 \rangle_{0,0} \langle H \rangle_{0,0} - \frac{1}{6} \langle RH \rangle_{0,0} \langle R^3 \rangle_{0,0} + \frac{1}{3} \langle R \rangle_{0,0} \langle H \rangle_{0,0} \langle R^3 \rangle_{0,0}
- \frac{1}{6} \langle R \rangle_{0,0} \langle R^3 H \rangle_{0,0} + \langle R \rangle_{0,0} \langle R^2 \rangle_{0,0} \langle RH \rangle_{0,0} - \frac{3}{2} \langle R \rangle_{0,0}^2 \langle R^2 \rangle_{0,0} \langle H \rangle_{0,0}
+ \frac{1}{2} \langle R \rangle_{0,0} \langle R^2 H \rangle_{0,0} - \frac{1}{4} \langle R^2 \rangle_{0,0} \langle R^2 H \rangle_{0,0} + \frac{1}{4} \langle R^2 \rangle_{0,0}^2 \langle H \rangle_{0,0}
- \langle R \rangle_{0,0}^3 \langle RH \rangle_{0,0} + \langle R \rangle_{0,0}^4 \langle H \rangle_{0,0}
+ O \left( \rho^5 \right). \quad (4.44)
$$

It should be noted that (4.44) contains terms up to the fourth order of $\rho$ and all expectation values are evaluated at vanishing chemical potential. This enables the use of the Potts model data of the $\mathbb{Z}_3$ spin model in terms of improved Taylor expansion. The susceptibility corresponding to (4.44) can be obtained by further derivation with respect to $J$.

**Polyakov Loop Susceptibility**

The Polyakov loop susceptibility can be obtained by applying (4.43) to (4.44) and reads

$$
\chi_{H\mu} = \langle H^2 \rangle_{0,0} - \langle H \rangle_{0,0}^2 
+ 2 \langle RH \rangle_{0,0}^2 - 2 \langle RH \rangle_{0,0} \langle H \rangle_{0,0} + 2 \langle R \rangle_{0,0} \langle H \rangle_{0,0}^2 - \langle R \rangle_{0,0} \langle H \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0}
+ \frac{1}{2} \langle R^2 H \rangle_{0,0}^2 - \langle R^2 \rangle_{0,0} \langle H \rangle_{0,0} + \langle R \rangle_{0,0} \langle H \rangle_{0,0} \langle R \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0}
- \langle RH \rangle_{0,0}^2 + 4 \langle RH \rangle_{0,0} \langle R \rangle_{0,0} \langle RH \rangle_{0,0} - \langle R \rangle_{0,0} \langle RH \rangle_{0,0}
- 3 \langle R \rangle_{0,0}^2 \langle H \rangle_{0,0}^2 + \langle R \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0}^2
+ \frac{1}{6} \langle R^3 H \rangle_{0,0}^2 - \frac{1}{3} \langle R^3 \rangle_{0,0} \langle H \rangle_{0,0}^2 + \frac{1}{3} \langle R^3 \rangle_{0,0}^2 \langle H \rangle_{0,0}^2 
$$

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\[ \begin{align*}
&- \frac{1}{6} \langle R^3 \rangle_{0,0} \langle H^2 \rangle_{0,0} - \frac{1}{2} \langle RH^2 \rangle_{0,0} \langle R^2 \rangle_{0,0} + 2 \langle RH \rangle_{0,0} \langle R^2 \rangle_{0,0} \langle H \rangle_{0,0} \\
&- \langle R^2 H \rangle_{0,0} \langle RH \rangle_{0,0} - 3 \langle R^2 \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0}^2 \\
&+ \langle R^2 \rangle_{0,0} \langle R \rangle_{0,0} \langle H^2 \rangle_{0,0} + \frac{3}{2} \langle R^2 H \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0} \\
&- \frac{1}{2} \langle R^2 H^2 \rangle_{0,0} \langle R \rangle_{0,0} + \frac{1}{2} \langle R^2 H \rangle_{0,0} \langle R \rangle_{0,0} \langle H \rangle_{0,0} + 2 \langle RH \rangle_{0,0} \langle R \rangle_{0,0} \\
&- \langle R \rangle_{0,0}^3 \langle H^2 \rangle_{0,0} \\
&+ O(\rho^4). \\
\end{align*} \tag{4.45} \]

It can be seen, that Equation (4.45) gives \( \chi_P \) at finite chemical potential in terms of the improved Taylor expansion up to the third order of \( \rho \).

Moreover, Equation (4.45) completes the calculation of observables in this section. The obtained results can be used for comparison with dual variable data, this will be done in the following.

4.2.3. Analysis of Observables in Terms of Improved Taylor Expansion

Since we want to compare the two Taylor expansions and also to the fugacity expansion outcome, the same statistics as in 2.5.3 and in 4.1.3 is taken for the assessment of the results based on the same statistics. This means all data points are for \( 10^6 \) measurements on \( 16^3 \) lattices in the following section. Moreover, the same values of \( \kappa \) are analyzed.

The final comparison of the two Taylor expansion methods and the fugacity expansion (for other values of \( \kappa \) and chemical potential) is conclusively dealt with in Chapter 5.

The following figures show how the orders of the improved Taylor series (ITE) add up to approach the flux representation results. This means the label ITE \( O(\mu^3) \) stands for the result of the sum up to third order of \( \mu \): \( O(\mu^0) + O(\mu^1) + O(\mu^2) + O(\mu^3) \), for example. First derivatives of the logarithm of the partition function (Polyakov loop and particle number) are computed and shown up to the fourth order of \( \mu \) and derivatives of second order of (4.15) are shown for \( \mu \) up to third order (Polyakov loop susceptibility and particle number susceptibility).

Following the conventions of 2.5.3, we begin our analysis with the comparison of the Polyakov loop (4.21) to the outcome of dual variable data for \( \kappa = 0.001 \).
4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

Figure 4.10.: Polyakov loop obtained in terms of improved Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to fourth order of $\rho$ (ITE $O(\rho^4)$, black) which are compared to flux representation results (red).

The improved Taylor expansion technique reproduces the Polyakov loop results at finite chemical potential - obtained in terms of dual variables - quite well, also for $\mu = 0.8$. This displays an advantage compared to the outcome of the regular Taylor expansion Figure 4.1. For the comparison of the ITE and the RTE, one has to match the results of the same orders of course, but the improved Taylor expansion shows also better agreement for $O(\rho^3)$ (magenta). Also the data points for the Polyakov loop at $\mu = 1$ show reasonable agreement.
4. Taylor Expansion Techniques

Figure 4.11.: Polyakov loop obtained in terms of improved Taylor expansion for $\kappa = 0.01$ as function of temperature. Shown are results up to fourth order of $\rho$ (ITE $O(\rho^4)$, black) which are compared to flux representation results (red).

Figure 4.11 shows that also the results in terms of dual variables for higher values of $\kappa$, specifically $\kappa = 0.01$ can be reproduced using improved Taylor expansion of fourth order of $\rho$. The outcome of the ITE at $\mu = 1$ in Figure 4.11 implies the increasing number of sharp bends in the coefficients of the Polyakov loop with increasing number of orders of $\rho$. The Polyakov loop obtained in terms of the improved Taylor expansion up to $O(\rho^4)$ (black) shows two kinks, whereas the results up to $O(\rho^3)$ (magenta) shows one. Nevertheless, the outcome for the Polyakov loop at $\mu = 1$ is reasonable at $\kappa = 0.01$. 

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Figure 4.12.: Polyakov loop susceptibility obtained in terms of improved Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to third order of $\rho$ ($\text{ITE } O(\rho^3)$, black) which are compared to flux representation results (red).

Since the second derivatives of the logarithm of the partition function are used to find the critical temperature and thus to exploit the phase diagram [7], it is advantageous, that the ITE is able to determine the critical temperature (and thus to determine $\chi_P$ sufficiently well) for $\mu$ up to 0.8 at least. At $\mu = 1$ it can be observed, that also the ITE suffers from the increasing minima and maxima when the chemical potential is enhanced, familiar from the regular Taylor expansion (Figure 4.3). It can further be noted, that the error bars get bigger as more orders are included. This is due to the fact that higher orders need a higher number of terms, which leads to larger fluctuations.
The Polyakov loop susceptibility at $\kappa = 0.01$ in terms of improved Taylor expansion agrees with the data of flux representation techniques up to $\mu = 0.8$. Convergence seems to be lost at $\mu = 1$, where the ITE up to fourth order of $\rho$ is not able to produce reliable data due to the additional minima and maxima and the progressive errors.
4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

The next observable in consideration is the particle number of the system.

![Graph with data points and lines showing quark number as a function of temperature for different chemical potentials.](image)

**Figure 4.14.** Quark number obtained in terms of improved Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to fourth order of $\rho$ (ITE $O(\rho^4)$, black) which are compared to flux representation results (red).

The quark number at $\kappa = 0.001$ obtained in terms of ITE shows very good agreement up to $\mu = 0.8$. The outcome at $\mu = 1$ in terms of the improved Taylor expansion is also acceptable, compared to the flux representation data.
The quark number at $\kappa = 0.01$ obtained in terms of ITE shows very good agreement up to $\mu = 0.8$. At $\mu = 1$, the particle number shows a kink near the phase transition. Nevertheless, the outcome of the particle number is quite reasonable, also for the higher value of the inverse mass parameter $\kappa$.
4.2. Improved Taylor Expansion for the $\mathbb{Z}_3$ Spin Model at Finite Chemical Potential

Figure 4.16.: Quark number susceptibility obtained in terms of improved Taylor expansion for $\kappa = 0.001$ as function of temperature. Shown are results up to fourth order of $\rho$ (ITE $O(\rho^4)$, black) which are compared to flux representation results (red).

Considering that the particle number susceptibility is a second derivative of the logarithm of the partition function, it can be expected, that the outcome for this observable is of the same quality as that of the Polyakov loop susceptibility. Even so, the results of the quark number susceptibility in terms of the improved Taylor expansion fail to reproduce dual variable data at $\mu = 0.8$ and at $\mu = 1$ the arising minima and maxima spoil the outcome (ITE $O(\rho^4)$).
4. Taylor Expansion Techniques

Figure 4.17: Quark number susceptibility obtained in terms of improved Taylor expansion for $\kappa = 0.01$ as function of temperature. Shown are results up to fourth order of $\rho$ (ITE $O(\rho^4)$, black) which are compared to flux representation results (red).

It can be expected, that the particle number susceptibility shows even worse results for higher values of $\kappa$, which is confirmed in Figure 4.17. Since the last added order makes the results for the particle number susceptibility unreliable, the improved Taylor expansion up to fourth order of chemical potential is not shown at $\mu = 0$ and $\mu = 1.8$. However, one should not forget that the results for the regular Taylor expansion shown in Figure 4.8 were of second order in $\mu$, therefore a direct comparison of the particle number susceptibility results in terms of the two treated Taylor expansion techniques is not advisable yet.

The final comparison of all three expansion techniques studied in this work will be performed in the following chapter.
5. Comparison of Expansion Techniques

So far, we tested Taylor and fugacity series expansion techniques concerning a small range of the chemical potential. At this point we show the phase diagram of the effective center model again, taking a closer look at it. The qualitatively behaviour,

![Phase diagram](image)

**Figure 5.1.:** Phase diagram of the effective center model for 4 values of $\kappa$ from \[7\] that the critical temperature decreases when the chemical potential is increased has already been reproduced in the former chapters of this work. An important point is here, that we work with the same units as in \[7\], that means a complete construction of the phase diagram requires the evaluation of observables up to $\mu \simeq 5$ for $\kappa = 0.01$, for example. This is possible in a representation without a sign problem (Figure 5.2).
5. Comparison of Expansion Techniques

Figure 5.2: Polyakov loop as a function of temperature and chemical potential obtained in terms of flux representation results at $\kappa = 0.01$ on a $36^3$ lattice [7].

We are now going to use the results obtained in terms of dual variables [7] as reference data to test the reliability and the limitations of Taylor- and fugacity series expansions in the effective center model. To this end we will increase the chemical potential until the complex action problem becomes severe and evaluate the Polyakov loop and its susceptibility in the critical temperature region. We are going to investigate the same values of $\kappa$ as in Figure 5.1. For these four values of $\kappa$, we already found that the complex action problem affects different regions of the chemical potential (Chapter 3) and that for higher values of $\mu$, smaller values of temperature are more affected.

It should be noticed, that all results obtained in terms of dual variables are from $10^6$ measurements, whereas the statistics for the expansion techniques varies.

Following the convention of the former chapters, we begin the comparison of all three expansion techniques with the observation of the Polyakov loop at $\kappa = 0.001$ (Figure 5.3).

The direct comparison of the two Taylor expansion techniques (Figure 5.3) shows the advantages of the improved Taylor expansion at $\mu = 0.8$. However, increasing the chemical potential further also leads to a breakdown of the ITE. At $\mu = 1.6$ one can see arising minima and maxima in the ITE outcome near the phase transition.

Figure 5.4 shows that additional orders do not improve convergence. Although the Taylor expansion techniques fail to produce reliable data for the first order derivative of the logarithm of the partition function at $\mu = 1.6$, the fugacity series gives reliable outcome until the complex action problem starts to get severe at $\mu = 3$ (Figure 3.1(a)).
Figure 5.3.: Polyakov loop as a function of temperature obtained in terms of Fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.001$. The results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1.6$. Fugacity expansion at $\mu > 1.6$ uses $4 \cdot 10^7$ measurements.
The next observable we consider is the Polyakov loop susceptibility in the critical temperature region at $\kappa = 0.001$ (Figure 5.7). The second derivatives show a behaviour similar to that of the first derivatives of the logarithm of the partition function. The Taylor expansion techniques fail even at small values of chemical potential to reproduce the Polyakov loop susceptibility near the crossover region and can therefore not be used to determine the critical temperature. The fugacity series is quite reliable until $\mu \geq 3$ it fails to converge.
Figure 5.5.: Polyakov loop susceptibility as a function of temperature obtained in terms of Fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.001$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1.6$. Fugacity expansion at $\mu > 1.6$ uses $4 \cdot 10^7$ measurements.
5. Comparison of Expansion Techniques

The following figures compare the 3 expansion techniques studied in this work to flux representation results at $\kappa = 0.01$. It could already be seen, that the region where the complex action problem becomes severe starts at $\mu = 1$. Beyond this value of chemical potential also increased statistics can not improve the outcome.

![Comparison of expansion techniques](image)

**Figure 5.6:** Polyakov loop as a function of temperature obtained in terms of Fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.01$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1$. Fugacity expansion at $\mu = 1.2$ uses $4 \cdot 10^7$ measurements.
Figure 5.7: Polyakov loop susceptibility as a function of temperature obtained in terms of Fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.01$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1$. Fugacity expansion at $\mu = 1.2$ uses $4 \cdot 10^7$ measurements.
5. Comparison of Expansion Techniques

To investigate the reliability and limitations of Taylor- and fugacity series expansions in the effective center model, we also consider the two further values of $\kappa$ for which the phase diagram was analyzed in Figure 5.1, namely $\kappa = 0.005$ and $\kappa = 0.1$, and determine the Polyakov loop and the corresponding susceptibility in the critical temperature region.

Continuing the analysis with the evaluation of observables at $\kappa = 0.005$, Figure 5.8 shows the Polyakov loop for various values of the chemical potential.

**Figure 5.8.** Polyakov loop as a function of temperature obtained in terms of fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.005$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1.2$. Fugacity expansion at $\mu = 1.6$ uses $10^7$ measurements.

Figure 5.8 shows how the expansion techniques are able to reproduce reliable data for small values of the chemical potential and how the Taylor expansion techniques fail to reproduce flux representation results in the region of the chemical potential where
the complex action problem is not dominating (Figure 3.2(a)), whereas the fugacity expansion gives reliable results for the Polyakov loop up to $\mu = 1.6$ where the complex action problem is prominent, especially for small values of $\tau$. A similar behaviour can be observed in the comparison of the outcome of the expansion techniques for the Polyakov loop susceptibility, Figure [5.9]. It should be mentioned that not all of the flux representation data points were reproduced at $\mu = 1.6$, since the failing of the fugacity series can be observed anyway.

Figure 5.9.: Polyakov loop susceptibility as a function of temperature obtained in terms of fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.005$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 1.2$. Fugacity expansion at $\mu = 1.6$ uses $10^7$ measurements.
5. Comparison of Expansion Techniques

The highest value of $\kappa$ analyzed in this thesis is $\kappa = 0.1$, for which Figure 3.2(b) showed, that the sign problem is severe even at small values of the chemical potential. Therefore, also the fugacity series can only reproduce flux representation results to a small extent (concerning $\mu$). It seems, that the improved Taylor series is in advantage of determining the critical temperature at $\mu = 0.5$.

![Polyakov loop as a function of temperature obtained in terms of fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.1$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 0.2$. Fugacity expansion and ITE at $\mu = 0.25$ and $\mu = 0.5$ use $10^7$ measurements.](image)

Figure 5.10.
Figure 5.11 shows that the improved Taylor expansion might determine the critical temperature better than the fugacity series for $\kappa = 0.1$ at $\mu = 0.25$. However, for $\mu = 0.5$ the improved Taylor expansion can not be used to determine $\tau_c$ (Figure 5.12).

Figure 5.11.: Polyakov loop susceptibility as a function of temperature obtained in terms of fugacity expansion (black), ITE (blue) and RTE (green) compared to flux representation results (red) at $\kappa = 0.1$. Results of expansion techniques up to third order of $\rho$ (ITE) and $\mu$ (RTE), respectively are shown. Flux representation results are from $10^6$ measurements as are expansion technique results for $\mu$ up to $\mu = 0.2$. Fugacity expansion and ITE at $\mu = 0.25$ use $10^7$ measurements.
Figure 5.12.: Polyakov loop susceptibility as a function of temperature obtained in terms of flux representation results at $\kappa = 0.1$ from $10^6$ measurements (red) compared to the outcome of ITE $O(\rho^3)$ from $10^7$ measurements (blue) at $\mu = 0.5$. 
6. Conclusion

The object of this thesis was the comparison of fugacity- and Taylor expansion regarding their ability of reproducing the phase diagram of the effective center model, a model theory for the center degrees of freedom of QCD. To this purpose, observables at finite chemical potential were calculated using fugacity expansion and two variants of Taylor expansion, referred to as regular and improved Taylor expansion. The results from these expansions were directly compared to results from simulations in the flux representation of the effective center model which allows Monte Carlo simulations at arbitrary chemical potential.

The transition from the confined phase to the deconfined phase was observed using the Polyakov loop as order parameter and the critical temperature could be extracted from the temperature dependence of the Polyakov loop susceptibility. Therefore the second derivatives of the logarithm of the partition function had to be accurately evaluated using series expansion techniques in order to reproduce the phase diagram.

In the previous study of the phase diagram of the effective center model four values of $\kappa$ were considered. $\kappa$ is a parameter which is proportional to the number of flavours and decreases with increasing particle mass. The same values of $\kappa$ were considered in this work for the comparison to the flux representation results.

It became apparent, that the fugacity expansion is not able to completely bypass the complex action problem, since the loss of convergence coincides with the region of chemical potential where the complex phase problem becomes severe. Nevertheless, this gives a relatively wide range of chemical potential values to explore for small $\kappa$, where the fugacity expansion is a suitable approach. In contrast, the regular Taylor expansion can only be used in a very small region of chemical potential values. The improved Taylor expansion performs somewhat better in this respect but also does not reach the range of chemical potential values accessible with the fugacity expansion.

The analysis of both Taylor expansion methods showed, that the increasing number of terms for higher order corrections also increase the error in the calculated observables. The fluctuations multiplied by powers of the chemical potential led to less reliable outcome when more orders were included for the evaluation of observables. The fugacity expansion does not have the issue of strongly fluctuating terms and in particular for small values of $\kappa$, the fugacity expansion shows great advantage compared to the two Taylor expansion methods.
6. Conclusion

For larger values of $\kappa$, the largest value we considered was $\kappa = 0.1$, the complex action problem is severe already at small values of the chemical potential, limiting the fugacity series due to the limited number of terms that can be evaluated sufficiently accurate. For this value of $\kappa$, the improved Taylor expansion slightly outperforms the fugacity series.

Neither the fugacity series nor the Taylor expansion techniques are able to reproduce the full phase diagram of the effective center model. Nevertheless, the assessment of the limitations and the region of reliability of both expansion techniques can be used to improve these methods for QCD.
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"We should all be thankful for those people who rekindle the inner spirit."

Albert Schweitzer

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