Non-Perturbative Aspects of Nonlinear Sigma Models

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von Raphael Flore M.Sc.
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Gutachter:

1. Prof. Dr. Andreas Wipf (Friedrich-Schiller-Universität Jena)
2. Prof. Dr. Martin Reuter (Johannes Gutenberg-Universität Mainz)
3. Prof. Dr. Roberto Percacci (SISSA, Trieste)

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1. Introduction

Quantum field theory (QFT) is a mathematical framework to describe the fundamental constituents and interactions of nature based on the physical principles of quantum mechanics and special relativity. It emerged in the investigations of electromagnetic interactions and was able to provide an impressingly accurate description of the physical observations [1, 2]. The applicability of the framework is yet not restricted to electrodynamics, but it was soon realized that the quantization of non-Abelian gauge theories [3] provides an appropriate mathematical description of strong [4] as well as weak interactions, while the latter one can be unified with electrodynamics to the electroweak interaction [5, 6, 7]. These two theories, the one of electroweak and the one of strong interactions (QCD), are the main building blocks of the Standard Model of particle physics, which describes the physical properties of all know fundamental particles.
A peculiar characteristic of nontrivial quantum field theories is the inevitable appearance of divergences. It was an important achievement in the development of QFT to formulate a renormalization procedure [8] which enables to remove these divergences. While this procedure is successful in many models (most prominently the Standard Model [9]), in some it is not, indicating that the corresponding description of the system can only be an effective one.
Most of the explicit computations of particle interactions and scattering amplitudes are performed by means of perturbation theory. While this approach is very successful in the analysis and prediction of high-energy collider experiments, it is not applicable to systems in which the couplings are large. Such systems, however, display some of the most interesting but yet not fully understood aspects of particle physics. The most prominent one is probably the confinement of quarks in color-neutral bound states [10, 11]. Despite many years of research there is still no sufficient theoretical analysis of the low-energy range of the QCD phase diagram. The deeper investigation of such phenomena requires a good command of efficient non-perturbative methods.
A further motiviation to develop non-perturbative tools is related to the long-lasting endeavor to find a quantum theory of gravitation. The theory of general relativity

can only be regarded as effective theory of gravity, because it is non-renormalizable from the point of view of perturbation theory. The existence of a nontrivial fixed point in parameter space, however, would establish the possibility that the theory is *asymptotically safe*, which means non-perturbatively renormalizable [12, 13].
The aim of this thesis is to investigate and further develop two non-perturbative methods, which have already been proven to be valuable tools for the investigations of field theories and which are applicable to a wide range of different phenomena: Lattice field theory [14] and the Functional Renormalization Group (FRG) [15]. The first approach relies on the discretization of field theories on (finite) spacetime lattices and enables to simulate the system by means of numerical computations that are usually performed by update algorithms like e.g. the Hybrid Monte Carlo algorithm [16]. The second approach implements the RG idea of gradual integration of momentum shells and provides a functional differential equation to describe the renormalization of an action functional which interpolates between the bare and the full effective action.
The FRG has been established as the primary tool[1] for the investigation of the asymptotic safety scenario [18]. The development of sophisticated computational techniques allows for studying increasingly large truncations of the effective action and convincing indications for the existence of a nontrivial fixed point could be found [19, 20, 21]. Nevertheless, further studies about the application of covariant FRG techniques to theories with nontrivial target space are required. A particular interesting question is if the results of the FRG concerning renormalization flows and the existence of nontrivial fixed points can be confirmed by another non-perturbative method like lattice field theory. These issues shall be discussed in Chap. 3 of thesis on the basis of a toy model.
The usual derivation of the FRG starts from the path integral representation of QFT which is formulated in terms of field configurations. An alternative to this Lagrangian formulation is given by the Hamiltonian description of quantum theories in terms of phase space variables, which is for example used in the canonical quantization of field theories. Arguments were brought forward recently that a Hamiltonian formulation of the FRG sheds light on nontrivial effects of the path integral measure [22]. Furthermore, it allows for alternative expansions of the truncation of the effective action [23], which could provide better access to some properties of nonlinear theories. Both suggestions shall be investigated in Chap. 4.
An interesting non-perturbative aspect of QCD besides the confinement is the still unsolved strong CP-problem [24]. It refers to fact that no violation of the CP sym-

[1]Another interesting approach in this direction are Causal Dynamical Triangulations [17].

metry has been observed in quantum chromodynamics so far, although the Standard Model would naturally allow for a term which breaks this symmetry. A mechanism is required which explains the suppression of such term. It is a topological operator which is invariant under small variations of the fields and one would hence expect that it is not affected by quantum fluctuations. Explicit calculations [25, 26, 27], however, showed that a more subtle analysis of the renormalization properties is necessary. In order to study this manifestly non-perturbative issue, the FRG should be an adequate tool and first computations in this framework have been performed for a generalization of the topological operator [28] with the interesting result that the topological parameter of Yang-Mills theories receives finite contributions from the extreme ultraviolet (UV) and extreme infrared (IR). A similar effect could be found in the IR of Cherns-Simons theory [29] and one may wonder if further models with topological term exhibit such renormalization properties. This shall be studied in Chap. 5 of this thesis.

Even if one could resolve the problems mentioned so far within the standard framework of quantum field theory, the Standard Model would still face some further challenges. The most prominent are the *hierarchy problem* of fine tuning in the Higgs sector [30], the missing explanation of dark matter [31], and the hope that electroweak and strong interactions may be unified at some high energy scale [32]. Various theories for physics “beyond the Standard Model” have been proposed [33], with supersymmetry [34] being one of the most influential ones among these. In order to investigate non-perturbative aspects of supersymmetric models, it would be desirable to have appropriate implementations on the lattice. However, supersymmetry is a nontrivial extension of the Poincaré symmetry [35] and hence broken by any spacetime discretization. To perform numerical simulations of supersymmetric theories is therefore an important, but nontrivial endeavor. It will be addressed in Chap. 6.

While all topics mentioned so far are related to the Standard Model or the theory of gravity, it is often advisable to study questions and computational methods first in their application to simpler toy models, as they can provide a more transparent view on conceptual aspects of the applied technique or the physical property. In this thesis the investigations will focus on nonlinear sigma models, which are the ideal testing ground to address the questions depicted above. Having a simpler structure than QCD or gravity, they yet share important features with these theories. Similar to gravity, nonlinear sigma models describe non-polynomial interactions and they have the same structure concerning power counting. With regard to QCD, sigma models can serve as toy model for most of the interesting properties of the theory like

asymptotic freedom, confinement, instantons or dynamical mass generation [36, 37]. An introduction to nonlinear sigma models will be given in Chap. 2, accompanied by a more detailed description of the applied non-perturbative approaches.
Note, that the computations in this thesis will be performed in Euclidean spacetime, if not stated otherwise. Furthermore, natural units are used, i.e. $\hbar$, c and k_B are set to one.

The compilation of this thesis is solely due to the author. However, parts of the work have been done in collaboration with colleagues from the research groups on quantum field theory in Jena, Bologna and Mainz. These collaborations are indicated at the beginning of the chapters.

2. The Models and the Methods

2.1. Nonlinear Sigma Models

Nonlinear sigma models (NLSM) are the theories of scalar fields ϕ which are maps from a d-dimensional spacetime Σ to a Riemann target manifold. The manifold is equipped with a metric $h_{ab}(\phi)$ and the fields can be regarded as coordinates on the target space. The microscopic action is defined as

$$S[\phi] = \frac{1}{2}\,\zeta \int d^dx\; h_{ab}(\phi)\,\partial_\mu\phi^a\,\partial^\mu\phi^b\,, \tag{2.1}$$

where ζ is a coupling constant. Note that usually the inverse parameter $g^2 = \zeta^{-1}$ is studied, while ζ is used in this thesis for the sake of convenience. It is natural to regard the fields ϕ^a as dimensionless, with the result that ζ has mass dimension $[\zeta] = d - 2$. The metric $h_{ab}(\phi)$ is a nontrivial function of the fields and encodes the (generically non-polynomial) interactions of these. It transforms as a symmetric 2-tensor, such that the action (2.1) is invariant under arbitrary reparametrizations $\phi \to \phi'(\phi)$ of the fields. Further symmetry properties of the NLSM are related to the isometries of the target manifold and hence depend on the specific model.
Since they were first introduced in particle physics [38], NLSM have become a versatile tool that is applied to a plethora of physical problems. It is impossible to cover all these applications and the related aspects of NLSM in this introduction in a comprehensive way. This means that some extensive and very interesting subjects have to be omitted, like for instance the rôle of NLSM in string theories, cf. [39] for an overview, or their use in effective theories of low-energy mesons and chiral perturbation theory [40]. This thesis will instead focus on two important classes of sigma models, the nonlinear $\mathrm{O}(N)$ models and the CP^n models. These are interesting in two dimensions as toy models for four-dimensional QCD [36] (sharing features like asymptotic freedom [41], dynamical mass generation and chiral symmetry breaking [37]), and in three dimensions in the description of statistical systems [42] as well as with regard to the concept of asymptotic safety [43]. Both classes of NLSM will be presented as bosonic theories in this chapter, while the supersymmetric extension of the nonlinear $\mathrm{O}(N)$ models will be discussed in Chap. 6.

2.2. Nonlinear O(N) Models

The target space of nonlinear O(N) models is the unit sphere in $\mathbb{R}^N$, i.e. the fields are maps $\phi : \Sigma \to S^{N-1}$. The field space of these maps will be denoted by $\mathcal{M}$. The target manifold is a homogeneous space $S^{N-1} = \mathrm{O}(N)/\mathrm{O}(N-1)$ whose isometry group is O(N). These isometries are generated by vector fields $K_i^a(\phi)$ which satisfy a generalized angular momentum algebra,

$$[K_i, K_j] = -f_{ij\ell} K_\ell \,, \tag{2.2}$$

where $f_{ij\ell}$ are the structure constants of the Lie algebra of the rotation group. The infinitesimal symmetries generated by the K_i are nonlinear

$$\phi^a \to \phi^a + \epsilon^i K_i^a(\phi). \tag{2.3}$$

From the invariant metric h_{ab} on the sphere one obtains the unique Levi-Civita connection Γ_{abc} and the corresponding

$$\text{Riemann tensor} \quad R_{abcd} = h_{ac}h_{bd} - h_{ad}h_{bc} \,, \tag{2.4}$$

$$\text{Ricci tensor} \quad R_{ab} = (N-2)\, h_{ab} \,, \qquad \text{and} \tag{2.5}$$

$$\text{scalar curvature} \quad R = (N-1)(N-2) \,. \tag{2.6}$$

The Levi-Civita connection on the sphere can be used to construct O(N)-covariant spacetime derivatives of the pullbacks of tensors on the sphere. For example, given a pullback of a vector on the sphere, its covariant derivative is

$$\nabla_\mu v^a \equiv \partial_\mu v^a + \Gamma^a{}_{bc} \partial_\mu \phi^b \, v^c \,. \tag{2.7}$$

The pullback covariant derivative ∇_μ will be used extensively in Chap. 3 and 5. The commutator of these covariant derivatives will be denoted by $H_{ab}^{\mu\nu}$ and its action on a vector of the sphere yields

$$H_{ab}^{\mu\nu} v^b = [\nabla^\mu, \nabla^\nu]_{ab}\, v^b = R_{abcd}\, \partial^\mu \phi^c \partial^\nu \phi^d \, v^b \,. \tag{2.8}$$

In this thesis two specific parametrizations will be used for some purposes: First, stereographic coordinates for which the metric reads

$$h_{ab} = \frac{1}{(1+\boldsymbol{\phi}^2)^2}\, \delta_{ab}, \tag{2.9}$$

where the fields ϕ^a are unconstrained $(N-1)$-tuple and $\boldsymbol{\phi}^2 = \sum_{a=1}^{N-1} \phi^a \phi^a$. Second, the representation in terms of N-tuples n^i which are explicitly constrained to the unit-sphere:

$$S[\boldsymbol{n}] = \frac{1}{2}\zeta \int d^d x \; \partial_\mu \boldsymbol{n} \partial^\mu \boldsymbol{n} \; , \quad \text{with } \boldsymbol{n}^2 = 1. \tag{2.10}$$

Both formulations are related by the stereographic projection and its inverse:

$$\begin{aligned} n^0 &= \frac{1-\boldsymbol{\phi}^2}{1+\boldsymbol{\phi}^2}, \; n^i = \frac{2\phi^i}{1+\boldsymbol{\phi}^2} \\ \phi^i &= \frac{n^i}{1+n^0} \qquad \text{for} \;\; i = 1, ..., N-1. \end{aligned} \tag{2.11}$$

In two dimensions the model is renormalizable and can be regarded as a fundamental theory. It is in fact integrable and the S-matrix could be derived in [44]. Based on this solution, the mass gap of the model could be computed [45] by comparing computations of the free energy that were obtained by the thermodynamic Bethe ansatz and by perturbation theory.

In constrast, nonlinear O(N) models in $d > 2$ are generally considered to be only effective theories, as the coupling constant has negative mass dimension[1] and the model is not perturbatively renormalizable. Nevertheless, small ϵ-expansions and RG-calculations show a phase transition and a related nontrivial fixed point of the renormalization flow in $d > 2$ [41, 46, 47, 43], which could render the theory non-perturbatively renormalizable, i.e. asymptotically safe. In the large-N limit this non-perturbative renormalizability could be proven rigorously [48]. For general N this question will be adressed in Chap. 3.

The critical properties of the phase transition in $d > 2$ are of great interest and have been intensively studied, since they describe the physical properties of a large range of systems: The effective theory in case of $N = 1$ corresponds to the Ising model, the case $N = 2$ to the XY-universality class and $N = 3$ to the Heisenberg model. But also models of larger N have interesting applications, like e.g. $N = 5$ being relevant in high-T_c superconductors [49]. And even the limit $N \to 0$ can be used in order to describe polymers dynamics by self-avoiding walks [50]. An extensive review about the applications of O(N) models in statistical physics is given in [42].

In this thesis it is understood that the O(N) universality class contains linear as well as nonlinear O(N) models, because it is generally assumed that both have the same critical properties. This assumpation is based on the hypothesis that two short-range theories in the same spacetime dimension and with the same symmetries belong to the same universality class. This statement is strongly supported in case of O(N)

[1] The relevant coupling in perturbation theory is $g^2 = \zeta^{-1}$.

models by many studies, cf. [51, 52, 53, 42, 54]. The extensive literature on the critical exponents of this universality class will provide useful benchmarks for the investigation of the methods applied in the following chapters. Finally, it should be stressed that all computations mentioned above indicate that the nontrivial fixed point of the theory only has one IR-relevant direction.

2.3. $\mathbf{CP}^n$ Models

The CP^n models are the theories of complex projective spaces. These are coset spaces $\mathrm{CP}^n = \mathrm{U}(n+1)/(\mathrm{U}(n)\times\mathrm{U}(1))$ whose isometry group is $\mathrm{PU}(n+1)$. They are Kähler manifolds and the corresponding potential can be written in terms of complex bosonic fields u^i with n components as $\log(1+\bar{\boldsymbol{u}}\boldsymbol{u})$, with $\bar{\boldsymbol{u}}\boldsymbol{u} = \sum \bar{u}^i u^i = |\boldsymbol{u}|^2$. The resulting Fubini-Study metric and the action of the model are given as

$$h_{a\bar{b}} = \frac{\delta_{ab}}{1+|\boldsymbol{u}|^2} - \frac{\bar{u}^a u^b}{(1+|\boldsymbol{u}|^2)^2} \tag{2.12}$$

$$S[\boldsymbol{u}] = \frac{1}{2}\zeta \int d^d x \; h_{a\bar{b}}(u)\, \partial_\mu u^a \partial^\mu \bar{u}^b \,. \tag{2.13}$$

Similar as in the $\mathrm{O}(N)$ models, it can often be useful to employ a formulation in terms of constrained fields z^i , $i = 0, ..., n$, with $\bar{\boldsymbol{z}}\boldsymbol{z} = 1$. The transformation between these two parametrizations reads

$$u^k = \frac{z^k}{z^0}\,, \quad \begin{pmatrix} z^0 \\ z^k \end{pmatrix} = \frac{\mathrm{e}^{i\alpha}}{(1+|\boldsymbol{u}|^2)^{1/2}} \begin{pmatrix} 1 \\ u^k \end{pmatrix}, \quad k = 1, ..., n\,. \tag{2.14}$$

The phase α accounts for the gauge freedom that arises from the additional field component which has two degrees of freedom of which only one is fixed by the constraint. The action (2.13) can be written in therms of the constrained fields by means of a covariant derivative as[2]

$$S[\boldsymbol{z}] = \frac{1}{2}\zeta \int d^d x \; \overline{D_\mu \boldsymbol{z}} D^\mu \boldsymbol{z}, \quad \text{with } D_\mu z^i = (\partial_\mu - \bar{\boldsymbol{z}}\partial_\mu \boldsymbol{z}) z^i. \tag{2.15}$$

The term $-\mathrm{i}\bar{\boldsymbol{z}}\partial_\mu \boldsymbol{z}$ can be interpreted as a gauge field A_μ, such that $D_\mu = \partial_\mu - \mathrm{i}A_\mu$, which transforms under the $\mathrm{U}(1)$ gauge transformation $\boldsymbol{z} \to \mathrm{e}^{\mathrm{i}\alpha(x)}\boldsymbol{z}$ as $A_\mu \to A_\mu + \partial_\mu \alpha$.

When CP^n models were first constructed [55, 56], it was immediately noted that their nontrivial topology allows for instantonic solutions in two dimensions. The

[2] up to an irrelevant numerical factor

different topologic sectors of the theory can be classified by the topological charge or "winding number"

$$Q = \frac{\mathrm{i}}{2\pi} \int d^2x \, \epsilon^{\mu\nu} \, \overline{D_\mu \boldsymbol{z}} D_\nu \boldsymbol{z} \, , \tag{2.16}$$

which assumes integer values for smooth field configurations. It provides a Bogomolnyi bound for the action:

$$0 \leq \int d^dx \; \overline{(D_\mu \boldsymbol{z} \pm \mathrm{i}\epsilon_{\mu\rho} D^\rho \boldsymbol{z})}(D^\mu \boldsymbol{z} \pm \mathrm{i}\epsilon^{\mu\sigma} D_\sigma \boldsymbol{z}) = 4\zeta^{-1} S \; \pm \; 2\mathrm{i} \int d^dx \; \epsilon^{\mu\nu} \, \overline{D_\mu \boldsymbol{z}} D_\nu \boldsymbol{z}$$

$$\Rightarrow S \geq \pi\zeta |Q|. \tag{2.17}$$

The existence of instantons is a feature that CP^n models share with QCD, providing a toy model in this respect, see e.g. [57]. A further similarity to QCD is, besides asymptotic freedom and a dynamically generated mass, the confinement of particles [58, 59]. More information about the use of CP^n models as toy models for strong interactions are given in [36, 60]. In addition, the models attracted interest in the field of supersymmetric field theories, since they naturally exhibit an extended supersymmetry due to their Kähler geometry [61]. This feature is, for instance, relevant in the study of supersymmetry on the lattice as it will be discussed in Chap. 6.

At the end of this introductory section about NLSM, the particularly interesting case $O(3) \cong \mathrm{CP}^1$ should be highlighted. The equivalence of nonlinear O(3) and CP^1 model can most easily be seen in terms of the constrained variables, in which the two alternative but yet equivalent formulations of the theory are related by the Hopf map

$$n^i = \boldsymbol{z}^\dagger \sigma^i \boldsymbol{z}, \;\; i = 1, 2, 3, \tag{2.18}$$

where σ^i denotes the Pauli matrices. Belonging to both classes of sigma models, the theory exhibits an especially rich structure. This thesis will deal with its supersymmetric properties and its lattice discretization (Chap. 6) as well as with the renormalization of the topological operator Q (Chap. 5).

2.4. Functional Renormalization Group

The effective action Γ is an efficient and comprehensive description of a physical theory, which serves as generator of all one-particle-irreducible (1PI) correlation functions. Based on the partition sum $Z[J]$ in the presence of an external source J and the corresponding generating functional of connected n-point functions, $W[J] = \log Z[J]$, the effective action can be defined as the Legendre transform

$$\Gamma[\phi] = \sup_J \big(J \cdot \phi - W[J] \big) . \tag{2.19}$$

The product $J \cdot \phi$ denotes the inner product of the Hilbert space, i.e. $\int d^d x \, J(x)\phi(x)$. Note that the discussion in this section solely deals with scalar fields, since this is sufficient for the purpose of this thesis. From (2.19) it follows immediately that

$$\phi = \frac{\delta W[J]}{\delta J} \quad \text{and} \quad \frac{\delta \Gamma[\phi]}{\delta \phi} = J . \tag{2.20}$$

The first equation states that ϕ is the expectation value of the quantum field (in the presence of the external source J), while the second relation represents a quantum version of the equations of motion. The definition (2.19) is equivalent to

$$\mathrm{e}^{-\Gamma[\phi]} = \int \mathcal{D}\varphi \; \mu[\varphi] \; \mathrm{e}^{-S[\varphi] - \frac{\delta\Gamma[\phi]}{\delta\phi} \cdot (\phi - \varphi)} . \tag{2.21}$$

While these basic concepts of quantum field theories are presented and discussed in more detail in standard text books like e.g. [62], the investigations in this thesis will focus on the renormalization properties of field theories. A powerful tool to study these is provided by the Renormalization Group (RG). The basic idea of the RG approach is to obtain an effective description of a physical system by reducing the number of degrees of freedom, either by averaging over subsets of these or (what is the same) by integrating out momentum shells, while the information from the substructure is incorporated in a redefinition $\{g_i\} \to \{g_i'\}$ of the physical parameters [63, 64, 65]. Note that, in principle, such an analysis has to consider all operators and corresponding couplings which can be generated, which are in general infinitely many.

Iterative infinitesimal RG transformations lead to a flow in the parameter space which describes the renormalization properties of the theory given by the beta functions of the couplings $\beta_{g_i}(\{g_j\})$. Of particular importance for the overall structure of such flows are the fixed points $\{g_i^*\}$ for which $\beta_{g_i}(\{g_j^*\}) = 0$. In the vicinity of these fixed points the beta functions can be linearized as

$$\beta_{g_i} = \sum_j M_i^j (g_j - g_j^*) + \mathcal{O}\big((g_j - g_j^*)^2\big) \quad \text{with} \quad M_i^j = \left.\frac{\partial \beta_{g_i}}{\partial g_i}\right|_{g=g^*} , \tag{2.22}$$

and the stability matrix M_i^j can be diagonalized as

$$M_i^j v_j^I = -\Theta^I v_i^I , \tag{2.23}$$

yielding the critical exponents Θ^I. The renormalization flow in the vicinity of a fixed point can then be written by means of these critical exponents as

$$g_i(k) = g_i^* + \sum_I g^I(k_0)\, v_i^I \left(\frac{k_0}{k}\right)^{\Theta^I} , \tag{2.24}$$

where the couplings at some scale k are determined by the couplings at some scale k_0 which are given in their decomposition $g^I(k_0)$ according to the basis of eigenvectors $\{v^I\}$. The directions in parameter space for which $\Theta_i > 0$ are amplified if one decreases the momentum scale k and are hence IR relevant, that means they are relevant in the macroscopic description of the system. A negative exponent $\Theta_i < 0$, in contrast, corresponds to an IR irrelevant direction, which is suppressed along the renormalization flow towards the IR. In case of $\Theta_i = 0$ the relevance of a direction cannot be decided from a linear approximation, but requires the investigation of higher orders of the expansion. A theory is renormalizable, i.e. a finite number of counter terms is sufficient to remove the divergences, if it contains a fixed point in the UV which has only a finite number of IR relevant directions. The search for such fixed points is the central issue in the asymptotic safety scenario [12].

A nontrivial fixed point with IR relevant direction indicates a second order phase transition in the model and the corresponding critical exponents of the physical observables are related to the exponents Θ of the renormalization flow. In this thesis the critical exponent ν of the correlation length in O(N) models will play an important rôle in the tests of FRG methods. If one considers the change of the correlation length along the relevant direction, it scales with $\frac{k}{k_0}$ under an RG transformation from scale k_0 to scale k. Comparing this behavior with the scaling of the relevant direction according to (2.24), it is straight forward to derive the relation between ν and the eigenvalue Θ^R corresponding to this direction:

$$\nu = \frac{1}{\Theta^R} . \tag{2.25}$$

A useful framework for the RG analysis of field theories is given by the Functional Renormalization group (FRG) [15]. It describes the renormalization flow of the Effective Average Action (EAA) Γ_k which depends on the momentum scale k and interpolates between the bare action at the UV-cutoff Λ and the full effective action in the IR:

$$\lim_{k\to\Lambda} \Gamma_k = S\,, \quad \lim_{k\to 0} \Gamma_k = \Gamma\,. \tag{2.26}$$

Note that the UV cutoff will henceforth be implicitly taken to infinity, i.e. it is assumed that this is possible and a related fundamental theory exists. The gradual integration of momentum shells as central idea of RG computations is implemented by the inclusion of a regulating term, usually called *cutoff action*,

$$\Delta S_k[\varphi] = \frac{1}{2}\int \frac{d^d q}{(2\pi)^d}\; \varphi(-q)\,\mathcal{R}_k(q^2)\,\varphi(q) \tag{2.27}$$

in the definition of the partition sum or directly in the integral expression of the effective action:

$$\mathrm{e}^{W_k} = Z_k[J] = \int \mathcal{D}\varphi\;\mu[\varphi]\;\mathrm{e}^{-S[\varphi]+J_k\cdot\varphi-\frac{1}{2}\varphi\cdot\mathcal{R}_k\varphi}\,, \tag{2.28}$$

$$\mathrm{e}^{-\Gamma_k[\phi]} = \int \mathcal{D}\varphi\;\mu[\varphi]\;\mathrm{e}^{-S[\varphi]-\frac{\delta\Gamma_k[\phi]}{\delta\phi}\cdot(\phi-\varphi)-\frac{1}{2}(\phi-\varphi)\cdot\mathcal{R}_k(\phi-\varphi)}\,. \tag{2.29}$$

The kernel $\mathcal{R}_k$ of the cutoff action is usually called *regulator* and is supposed to suppress the low-energy modes $\varphi(p)$ with $|p| < k$, such that the path integral in effect integrates out only the high-energy modes, leading to an effective action for the low-energy system. In order to provide the correct interpolation of the EAA the regulator has to fulfill the following properties:

$$1.\ \lim_{q^2/k^2\to 0} \mathcal{R}_k(q^2) > 0, \quad 2.\ \lim_{k^2/q^2\to 0} \mathcal{R}_k(q^2) = 0, \quad 3.\ \lim_{k^2\to\infty} \mathcal{R}_k(q^2) \to \infty\,. \tag{2.30}$$

The third requirement ensures $\lim_{k\to\Lambda}\Gamma_k = S$, as the cutoff action in (2.29) becomes a dominant Gaußian integral which leads to $\delta(\phi-\varphi)$. Note that the general structure of the regulator is $\mathcal{R}_k(z) = z\; r(z/k^2)$, as suggested by a dimensional analysis. Note also that it is often more reasonable, from a physical or computational point of view, to coarse-grain w.r.t. a covariant Laplacian or another kinetic operator instead of the flat derivative $-\partial^2$.

The definition of the EEA given by the path integral in (2.29) coincides with a modified Legendre transform

$$\Gamma_k[\phi] = \sup_J \big(J \cdot \phi - W_k[J]\big) - \Delta S_k[\phi] \tag{2.31}$$

$$\Rightarrow \phi(x) = \frac{\delta W_k[J]}{\delta J(x)}, \quad J(x) = \frac{\delta \Gamma_k[\phi]}{\delta \phi(x)} + (\mathcal{R}_k \phi)(x)\,. \tag{2.32}$$

The FRG scheme is a particular powerful tool to investigate the renormalization of theories, because it provides an exact and concise formula for the evolution of the effective (average) action [15]. This *flow equation* can be derived from (2.29) or (2.31) by taking the derivative $k\,\partial_k$ and using the relations (2.32). The derivation can be found in references like e.g. [66] and it will not be repeated here. Instead, the derivation of a similar flow equation will be presented in Chap. 4.2 and should illustrate the general reasoning. The flow equation for the EAA reads:

$$k\partial_k \,\Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\left\{k\partial_k \mathcal{R}_k \left(\mathcal{R}_k + \Gamma_k^{(2)}[\phi]\right)^{-1}\right\}\,. \tag{2.33}$$

Some remarkable features of this equation shall be highlighted: In contrast to the standard formulation of QFT in terms of functional integrals, the FRG scheme is based on a functional differential equation, which improves the accessibility for computations. Furthermore, (2.33) has a simple one-loop structure, written in terms of the propagator $G_k = (R_k + \Gamma_k^{(2)})^{-1}$. The flow equation is yet an exact equation which takes non-perturbative effects into account. In fact, one could regard (2.33) in combination with initial conditions in the UV as the defining prescription of quantum field theories, which already contains an appropriate regularization. By construction, $\mathcal{R}_k$ ensures the regularization of the IR modes, but it even provides a UV regularization if it is chosen such that the derivative $k\partial_k\mathcal{R}_k(q^2)$ in the numerator of (2.33) falls off sufficiently fast for $q^2 \to \infty$. The exact flow of the EAA through coupling space obviously depends on the specific choice of $\mathcal{R}_k$, as computations in QFT generally depend on the regularization scheme. But the resulting full effective action and hence the physical observables are independent of $\mathcal{R}_k$.
However, leaving this conceptual point of view and turning towards explicit calculations, one encounters the problem that the renormalization flow will in general generate all possible operators that are compatible with the symmetries of the system, which are usually infinitely many. Since it is impossible to handle such expressions in analytical or numerical calculations, one has to employ approximations which consist of truncating the effective action at a certain order of a systematic expansion. The two most common expansion schemes are the *vertex expansion* in powers of interacting fields and the *derivative expansion* in powers of momenta. This thesis will only

address the second scheme. Because of the increasing mass dimension of the higher-order operators, the canonical mass dimension of the related couplings decreases and one expects that they become less and less relevant. This argument, however, holds only true if the anomalous dimension is small. Furthermore, one should always keep in mind that the applied truncations are an approximation scheme that is not fully under control and in which the impact of higher-order operators can hardly be predicted.

Another disadvantage of the necessary truncations is that the results become regulator-dependent. For reasonable regulators the deviations should be rather small and not affect the qualitative results. Where a specification of the regulator is necessary in this thesis, adapted variants of the *optimized regulator* will be used, whose basic structure reads [67, 68, 69]

$$\mathcal{R}_k \propto (k^2 - p^2)\,\Theta(k^2 - p^2)\,, \tag{2.34}$$

with $\Theta(x)$ being the Heaviside step function. The aim of this chapter was to present the basic concepts and features of the FRG approach to QFT. More detailed information and discussions can be found in [70, 71, 72, 73, 66, 74]. Since its first derivation twenty years ago [15] the FRG formalism has been successfully applied to many problems in very different subjects, ranging from gauge theories [75, 66] over condensed matter systems [76] and statistical physics [70] to gravity [18, 20]. This thesis will employ the FRG in order to investigate the renormalization of topological charges (Chap. 5), to develop and investigate alternative functional RG schemes based on a Hamiltonian formulation of QFT (Chap. 4), and to obtain a covariant analysis of the three-dimensional nonlinear $\mathrm{O}(N)$ models (Chap. 3).

Concerning the notation, the scale derivative $k\partial_k$ was already introduced. In terms of the logarithm $t \equiv \log(k/\Lambda)$ it can be written as ∂_t and further abbreviated as $\partial_t O_k = \dot{O}_k$ in its application to any k-dependent object O. Note that the beta function β_g of a coupling g is directly given by $\dot{g}$. The different representations of the derivatives and beta functions will be used interchangeably in this thesis.

2.5. Lattice Field Theory

An alternative and very popular approach to investigate quantum field theories and their non-perturbative aspects is provided by numerical simulations of corresponding lattice field theories. The starting point is the discretization of the quantum theory on a finite spacetime lattice G:

$$G = \left\{ x = (x_1, ..., x_d) = a(n_1, ..., n_d) \mid n_i = 0, ..., N_i - 1;\, i = 1, ..., d \right\}, \tag{2.35}$$

where N_i denote the lattice extent, i.e. the number of lattice sites along the spacetime direction i, and a is the lattice spacing[3]. This discretization naturally provides a regularization of the theory by introducing cutoffs Λ and λ in the UV and the IR respectively. No fluctuations below the fundamental lattice spacing can be resolved such that the momenta in the computation are bounded from above by the size of the Brillouin zone. In the IR the modes are bounded from below by the total physical extent $L_i = aN_i$ of the lattice[4]:

$$\Lambda = \frac{\pi}{a}, \quad \lambda = \frac{\pi}{L} = \frac{\pi}{Na}. \tag{2.36}$$

By means of this lattice regularization the path integral becomes a well-defined expression which consists of a finite number of integrations:

$$\mathcal{Z} = \int \mathcal{D}\phi \; \mu(\phi) \; \mathrm{e}^{-S[\phi]} \Longrightarrow \int \prod_{x \in G} d\phi_x \; \mu(\phi_x) \, \mathrm{e}^{-S_{disc}[\phi_x]}. \tag{2.37}$$

The discretization of the action functional is not unique, but different discretizations can correspond to the same continuum limit. Especially the discretization of the derivative operators allows for several different prescriptions, which have specific advantages and disadvantages and should be adjusted to the physical problem studied.

Each of these regularizations is affected by lattice artefacts which depend on the finite spacing a. In order to obtain the universal properties of a system, one has to consider the continuum limit $a \to 0$. In case of a fixed lattice extent N_i, however, this limit leads to a continuous but vanishing physical space, which does not provide reasonable information. It is therefore important to keep the physical volumne fixed by increasing N_i while decreasing a.

A crucial aspect of the discretization of field theories is the treatment of symmetries.

[3]Note that lattice computations usually do not have an intrinsic length scale, but the physical size has to be measured against reference masses that can be determined from correlation functions.

[4]In this thesis only lattices with equal extent in all dimensions will be considered.

The Poincaré group of continuous spacetime symmetries is obviously broken down to a discrete subgroup. But while this symmetry is, by construction, fully restored in the continuum limit, the discretization induced breaking of other symmetries can persist in the continuum limit, if it generates operators which are relevant with regard to renormalization. One prominent example of such symmetry breaking on the lattice is supersymmetry, which will be discussed in more detail in Chap. 6.
Even though the path integral is strongly simplified by the lattice discretization (2.37), it still constitutes the weighted sum of infinitely many configurations. However, since most of these configurations are exponentially suppressed, *importance sampling* can be used in order to improve the computations and distribute the sampling points efficiently according to the weighting factor e^{-S}. A particular powerful realization of importance sampling is the Hybrid Monte Carlo (HMC) algorithm [16], which is a combination of molecular dynamics [77] and Metropolis algorithm [78]. These algorithms are described in many standard text books like [14] and will not be presented here. This thesis will not deal with the details or implementations of numerical simulations, but rather concentrates on a discussion of the discretization of supersymmetric models (Chap. 6) and on the possibility to determine the renormalization flow of nonlinear theories from lattice computations (Chap. 3.5).

3. Fourth-Order Derivative Expansion of Nonlinear O(N) Models

The calculations presented in Sec. 3.2 - 3.4 were performed in collaboration with Omar Zanusso and Andreas Wipf and have already been published in [79]; Sec. 3.5 depicts the results of a collaboration with Daniel Körner and Björn Wellegehausen.

The Functional Renormalization Group and the lattice approach are two complementary and very distinct non-perturbative methods of quantum field theory. Although they are both applicable to a wide range of phenomena, there is only limited information about a direct comparison of these two approaches. The intention of this chapter is to provide an investigation of the flow diagram of three-dimensional nonlinear O(N) models in a fourth-order derivative expansion by means of the FRG as well as the Monte Carlo Renormalization Group. Nonlinear O(N) models in three dimensions are an interesting field for this endeavor considering the possibility of non-perturbative renormalizibality owing to the existence of a nontrivial fixed point. Furthermore, these models have attracted a lot of attention within statistical field theory, so that their critical properties are well-studied, see e.g. [42, 52, 53, 80, 81, 82], and can serve as benchmarks for the analysis of the methods. Finally, it is reasonable to start the investigation of flow diagrams by means of the Monte Carlo Renormalization Group in theories like purely bosonic O(N) models which can be simulated by HMC algorithms with a feasible computational effort.

3.1. The Nonlinear Model as a Limit of the Linear Model

Starting with the investigation by means of the FRG, one may first study the detailed results about the linear O(N) models which were obtained within this framework [70]. On the level of the classical action, the nonlinear model can be deduced as a particular limit of the linear one in which the bare potential $V(\phi)$ becomes infinitely steep and confines the field configurations to $\phi^2 = \kappa$, i.e. to a sphere with some radius $\kappa^{1/2}$. If one adopts this perspective on the nonlinear model and consider renormalization, one could assume that the limit corresponding to this model is just a specific, unstable point in parameter space which flows to an effective linear model. While it is generally excepted that both theories belong to the same universality class as explained in Chap. 2, this question has not been clearified so far. In fact, it is still questionable, whether the limit of the linear model is on the level of a quantum theory really equivalent to the nonlinear one, although there have been positive indications in this respect [54].

In this section it shall be assumed that the nonlinear model can indeed be regarded as such limit in order to see what one can learn about the renormalization properties. A simple truncation of the linear model which has been studied by FRG methods [70] reads

$$\Gamma_k[\phi] = \frac{1}{2} \int d^d x \, Z_k \, \partial_\mu \phi \partial^\mu \phi + \lambda_k (\rho - \kappa_k)^2 \,, \tag{3.1}$$

where $\rho = \frac{1}{2}\phi^a \phi_a$, and $\phi \in \mathbb{R}^N$. The transition to a simple truncation of the nonlinear model according to (2.10) is given by a rescaling of the fields such that $\zeta_k = 2 Z_k \bar{\rho}_k$ and by taking the limit $\lambda_k \to \infty$. The running of the dimensionless coupling $\tilde{\zeta}$ is derived in [70] and in case of an optimized regulator (2.34) its limit for $\lambda \to \infty$ is given as

$$\partial_t \tilde{\zeta} = (2-d)\, \tilde{\zeta} + 2(N-2)\, c_d \,, \tag{3.2}$$

where $c_d = \left((4\pi)^{d/2} \Gamma[d/2+1] \right)^{-1}$. This result exactly coincides with a covariant computation for the nonlinear model, as it was already pointed out in [43], and it furthermore agrees (up to a numerical factor) with one-loop calculations [51]. While the beta function in $d > 2$ has a nontrivial fixed point at $\tilde{\zeta}^* = \frac{2(N-2)c_d}{d-2}$ in favor of non-perturbative renormalizibility, the utilized approximation is not sensitive to the critical properties of the related phase transition, which depend on N, i.e. on the dimensionality of the target manifold. For instance, a computation of the critical exponent ν based on (3.2) leads to $\nu = 1/(d-2)$ for all N, which is the expected exponent only for $N \to \infty$.

The FRG analysis in [70] also states the beta function of the dimensionless coupling $\tilde{\lambda}_k$, from which one can deduce the running of its inverse by using an optimized regulator:

$$\partial_t \tilde{\lambda}^{-1} = -\frac{\partial_t \tilde{\lambda}}{\tilde{\lambda}^2} = -\left(d - 4 - 2\frac{\partial_t Z}{Z} \right) \tilde{\lambda}^{-1} + \frac{c_d}{2} \left(\frac{9}{(1+\tilde{\lambda}\tilde{\zeta})^3} + (N-1) \right) \tag{3.3}$$

which has no fixed point at $\lambda^{-1} = 0$, but is $\frac{c_d}{2}(N-1)$, which means that the infinitely steep potential at the UV smoothen out towards the IR. This seems to support the idea that the bare nonlinear theory really flows towards an effective linear theory. However, this finding should not be overemphasized and one would need to include further operators in order to get a decisive answer to this question.
The natural next order in an expansion of the truncation would be the introduction of a nontrivial wave function renormalization $Z_k(\phi)$. Such a truncation was considered in [83], supported by a more detailed analysis of $\partial_t Z_k(\phi)$ in the appendix of [84]. Studying the results one notices that the enhancement of the wave function renormalization neither changes the arguments concerning $\partial_t \tilde{\lambda}^{-1}$ nor improves the critical properties, since all relevant N-dependent terms are still suppressed in the limit $\lambda \to \infty$. In fact, it is not suprising that the N-dependence is extinguished by this limit in any FRG computation that is based on a truncation of second order in the derivatives, if one considers the results of [43] which were obtained for a covariant ansatz for a generic class of nonlinear sigma models. In a simple second-order derivative expansion, the resulting beta function has the same structure for all different models. The distinct characteristic properties will become relevant only in the next order of the derivative expansion, as it depends on the symmetries of the specific model which terms have to be included at this order.
Fourth-order calculations in the linear model become quite involved due to the large variety of possible operators. Such a computation has been executed [85], but leads to very complicated expressions such that it becomes unfeasible to perform the appropriate limit and gain information about the nonlinear model[1]. It is therefore more reasonable to work directly in a manifestly nonlinear formulation.

3.2. Covariant Nonlinear Analysis

The nonlinear geometry of the theory was already described in Chap. 2 and the motivation of this chapter is to investigate the renormalization and the critical properties of the model by a manifestly covariant method within the FRG framework, which does not rely on an embedding of the theory in a linear space or on an explicit breaking of symmetries , but respects the geometrical properties at each step of the calculation. Appropriate techniques which rely on a combination of a covariant background field expansion and the heat kernel method have already been developed and applied to NLSM [43, 86, 87, 88, 89], with a focus on chiral SU(N) models. These

[1] More detailed information about the calculations was kindly provided by D. Litim, but they still remained impracticable.

techniques shall be investigated further in this section in a fourth-order derivative expansion of nonlinear $\mathrm{O}(N)$ models. Note that the formalism will first be derived for a general spacetime dimension, before the results will be discussed in more detail in $d = 3$.
The most general ansatz for an effective average action up to fourth order in the derivatives which respects the isometries of the model is given as[2]

$$\Gamma_k^{\mathrm{s}}[\phi] = \frac{1}{2}\int d^dx \; \zeta_k \, h_{ab} \, \partial_\mu\phi^a\partial^\mu\phi^b + \alpha_k \, h_{ab} \, \Box\phi^a\Box\phi^b + T_{abcd} \, \partial_\mu\phi^a\partial^\mu\phi^b \, \partial_\nu\phi^c\partial^\nu\phi^d \, . \quad (3.4)$$

The square of the covariant derivative (2.7) is denoted by $\Box \equiv \delta^{\mu\nu}\nabla_\mu\nabla_\nu$ (acting on ϕ^a it yields $\Box\phi^a = \nabla_\mu\partial^\mu\phi^a$) and $\Delta = -\Box$. The tensor T_{abcd} fulfills the symmetry relation $T_{abcd} = T_{((ab)(cd))}$ and can be parametrized without loss of generality as

$$T_{abcd} \;\; = \;\; L_{1,k}h_{a(c}h_{d)b} + L_{2,k}h_{ab}h_{cd} \, , \quad (3.5)$$

since h_{ab} is (up to normalization) the unique invariant 2-tensor in the simple case of nonlinear $\mathrm{O}(N)$ models, and all invariant tensors of higher rank can be constructed from h_{ab}. Using this parametrization, the ansatz (3.4) for the EAA contains four couplings: $\{\zeta_k, \alpha_k, L_{1,k}, L_{2,k}\}$. They parametrize the set of included operators and encode the explicit k-dependence of Γ_k.
In order to develop a covariant analysis of the FRG flow equation for this ansatz, an appropriate background field expansion of the action functional (3.4) should be constructed, which maintains the nonlinear symmetries of the theory. Note that the metric $h_{ab}(\phi)$ can be understood as metric $h_{ab}(\phi)$ on field space $\mathcal{M}$ where trivial spacetime indices have been suppressed for brevity. In a similar manner, the Levi-Civita connection, the curvature tensors and the Laplacian can be promoted to $\mathcal{M}$ as well [90]. It is a crucial point of the expansion procedure that the expansion variable ought to possess well-defined transformation properties both in the background field φ^a and in the full field ϕ^a. It would be, for instance, a particularly hard task to construct $\mathrm{O}(N)$ covariant functionals in terms of the difference $\phi^a - \varphi^a$ of two points in field space as it transforms neither like a scalar, nor like a vector under isometries. For ϕ being in a sufficiently small neighbor of φ, there exists a unique geodesic in $\mathcal{M}$ connecting φ and ϕ, which enables to construct the *exponential map*

$$\phi^a = \mathrm{Exp}_\varphi \xi^a = \phi^a(\varphi, \xi) \, . \quad (3.6)$$

[2]The meaning of the superscript s will become clear in the context of the background field expansion and the consequent distinction between "single-field" and "bi-field" action.

Here, ξ is an implicitly defined vector that belongs to the tangent space of $\mathcal{M}$ at φ. Moreover, ξ is a bi-tensor, in the sense that it has definite transformation properties under φ^a as well as ϕ^a transformations. For this reason it can be understood as $\xi^a = \xi^a(\varphi, \phi)$. It transforms as a vector under the O(N) transformations of φ^a and as a scalar under those of ϕ^a. By construction, the norm of ξ equals the distance between φ and ϕ in $\mathcal{M}$ [39]. The definite transformation properties make ξ a candidate to parametrize any expansion of functionals of the kind $F[\phi]$ around a background φ.

The expansion of the action (3.4) can now be performed in a fully covariant way by introducing the affine parameter $\lambda \in [0, 1]$ that parametrizes the unique geodesic connecting φ and ϕ [91, 39]. Let φ_λ be this geodesic with $\varphi_0 = \varphi$ and $\varphi_1 = \phi$, and let $\xi_\lambda = d\varphi_\lambda/d\lambda$ be the tangent vector to the geodesic at the generic point φ_λ. One can introduce the derivative along the geodesic $\nabla_\lambda \equiv \xi^a_\lambda \nabla_a$, for which $\nabla_\lambda \xi^a_\lambda = 0$ and $\nabla_\lambda h_{ab} = 0$. Its relation to the pullback derivative is

$$\nabla_\lambda \partial_\mu \varphi^a_\lambda = \nabla_\mu \, \xi^a_\lambda \,. \tag{3.7}$$

The commutator of the the covariant derivatives ∇_λ and ∇_μ can be computed on the pullback of a generic tangent vector v^a,

$$[\nabla_\lambda, \nabla_\mu] v^a = R_{cd}{}^a{}_b(\varphi_\lambda)\, \xi^c \, \partial_\mu \varphi^d_\lambda \, v^b \,. \tag{3.8}$$

The expansion of a functional $F[\phi]$ can now be performed on the basis of ∇_λ, if one regards $F[\phi]$ as the limit $\lambda \to 1$ of $F[\varphi_\lambda]$, and expands the latter in powers of λ around $\lambda = 0$. Using the fact that $F[\phi]$ is scalar function of ϕ, this expansion reads

$$F[\phi] = \sum_{n\geq 0} \frac{1}{n!} \frac{d^n}{d\lambda^n} F[\varphi_\lambda] \bigg|_{\lambda=0} = \sum_{n\geq 0} \frac{1}{n!} \nabla^n_\lambda F[\varphi_\lambda] \bigg|_{\lambda=0} \,, \tag{3.9}$$

and yields a power series in ξ^a:

$$F[\phi] = \sum_{n\geq 0} F^n_{(a_1,\ldots,a_n)}[\varphi] \, \xi^{a_1} \ldots \xi^{a_n} \,. \tag{3.10}$$

If one applies this procedure to (3.4), the second order of $\Gamma^{\mathrm{s}}_k[\phi] = \Gamma^{\mathrm{s}}_k[\varphi, \xi]$ in ξ, which will be relevant in the subsequent computations, reads:

$$
\begin{aligned}
&\Gamma^{\mathrm{s}}_k[\varphi,\xi]|_{\xi^2} = \\
&\tfrac{1}{2}\int d^d x\; \zeta_k h_{ab}\nabla_\mu\xi^a\nabla^\mu\xi^b - \zeta_k R_{acbd}\partial_\mu\phi^c\partial^\mu\phi^d\xi^a\xi^b + 2\alpha_k R_{acbd}\partial_\mu\phi^c\partial^\mu\phi^d\xi^a\Box\xi^b \\
&\qquad + \alpha_k h_{ab}\Box\xi^a\Box\xi^b + \alpha_k R_{abcd}R^a{}_{efg}\partial_\mu\phi^b\partial^\mu\phi^d\partial_\nu\phi^e\partial^\nu\phi^g\xi^c\xi^f + \alpha_k R_{abcd}\Box\phi^a\Box\phi^d\xi^b\xi^c \\
&\qquad + \alpha_k R_{abcd}\Box\phi^a\partial_\mu\phi^d\xi^b\nabla^\mu\xi^c + \alpha_k R_{abcd}\Box\phi^a\partial_\mu\phi^b\xi^c\nabla^\mu\xi^d + 3\alpha_k R_{abcd}\Box\phi^a\partial_\mu\phi^d\xi^c\nabla^\mu\xi^b \\
&\qquad + 2T_{abcd}\nabla_\mu\xi^a\nabla^\mu\xi^b\partial_\nu\phi^c\partial^\nu\phi^d + 4T_{acbd}\nabla_\mu\xi^a\nabla_\nu\xi^b\partial^\mu\phi^c\partial^\nu\phi^d \\
&\qquad - 2R_{abcd}T^a{}_{efg}\partial_\mu\phi^c\partial^\mu\phi^e\partial_\nu\phi^f\partial^\nu\phi^g\xi^b\xi^d\;. \qquad (3.11)
\end{aligned}
$$

Note that the covariant derivative ∇_μ (2.7) and the tensors h_{ab}, R_{abcd} and T_{abcd} are here and in the following evaluated at the base point φ.
The defining functional integral of the effective average action was already explained in (2.29). In the background field formalism it reads:

$$
e^{-\Gamma_k[\varphi,\xi]} = \int \mathcal{D}\xi'\,\mu[\varphi]\,\mathrm{e}^{-S[\varphi,\xi'] - \frac{\delta\Gamma_k}{\delta\xi^a}[\varphi,\xi]\cdot(\xi^a - \xi'^a) - \Delta S_k[\varphi,\xi-\xi']}\,, \qquad (3.12)
$$

where ξ' denotes the quantum degrees of freedom which are the variables of the bare action, while the fields ξ and ϕ are average fields and the variables of the EAA. The cutoff action has to be a covariant functional which regularizes the fluctuation fields ξ' and ξ. The appropriate form is

$$
\Delta S_k[\varphi,\xi] = \frac{1}{2}\int d^d x\;\xi^a\mathcal{R}^k_{ab}(\varphi)\xi^b\,, \qquad (3.13)
$$

where $\mathcal{R}_{ab}(\varphi)$ is some symmetric 2-tensor which depends on the base point φ^a. The functional (3.13) is invariant under transformations of the background field φ^a as well as of the field ϕ^a.
The running of the EAA can be derived from (3.12) in the usual way as

$$
k\partial_k\Gamma_k[\varphi,\xi] = \frac{1}{2}\,\mathrm{Tr}\left(\frac{k\partial_k\mathcal{R}_k(\varphi)}{\Gamma^{(0,2)}_k[\varphi,\xi] + \mathcal{R}_k(\varphi)}\right)\,. \qquad (3.14)
$$

Functionals of the kind $F[\phi]$ are never genuine functions of two fields, but rather a function of the single combination $\phi^a(\varphi,\xi)$ and may therefore be called *single-field* functionals. For general $\mathcal{R}_{ab}(\varphi)$, there is however no evident way to recast (3.13) as a functional of the single field ϕ^a. Functionals like (3.13) are genuine functions of φ and ξ independently and may be called *bi-field* functionals. The consequence of such cutoff action is that the effective average action $\Gamma_k[\varphi,\xi]$ also becomes a bi-field functional [92, 93, 94, 95]:

$$\hat{\Gamma}_k[\varphi,\phi] = \Gamma_k[\varphi,\xi(\varphi,\phi)]\,. \tag{3.15}$$

This observation is important in order to understand that the only way to obtain a single field effective action from this is to set $\varphi = \phi$ or equivalently $\xi = 0$ and consider

$$\bar{\Gamma}_k[\phi] = \hat{\Gamma}_k[\phi,\phi] = \Gamma_k[\phi,0]\,. \tag{3.16}$$

The limit $k \to 0$ of $\bar{\Gamma}_k[\phi]$ coincides with the well known effective action introduced by deWitt [96].
In order to account for the bi-field structure of $\Gamma_k[\varphi,\xi]$, the single-field ansatz (3.4) has to be extended by a bi-field functional $\Gamma^{\mathrm{b}}_k[\varphi,\xi]$,

$$\Gamma_k[\varphi,\xi] \;\;=\;\; \Gamma^{\mathrm{s}}_k[\phi(\varphi,\xi)] + \Gamma^{\mathrm{b}}_k[\varphi,\xi]\,, \tag{3.17}$$

for which $\Gamma^{\mathrm{b}}_k[\varphi,0] = 0$. It should be chosen such that the 2-point function of the field ξ^a is dressed appropriatly, because it is the second derivative w.r.t. ξ which determines the flow (3.14). The choice studied here is

$$\Gamma^{\mathrm{b}}_k[\varphi,\xi] = \Gamma^{\mathrm{s}}_k[\phi(\varphi,Z_k^{1/2}\xi)] - \Gamma^{\mathrm{s}}_k[\phi(\varphi,\xi)] + Z_k\frac{m_k^2}{2}\int d^dx\; h_{ab}\xi^a\xi^b\,. \tag{3.18}$$

It introduces a mass term for the fluctuation fields as well as a nontrivial wave function renormalization of these fields $\xi^a \to Z_k^{1/2}\xi^a$, which takes into account the possibility that the fields φ^a and ξ^a may have different scaling behaviors. In a first step beyond the covariant gradient expansion it is assumed that Z_k is field independent. It will become obvious later that the wave function renormalization enters the flow solely via the anomalous dimension $\eta_k = -\dot{Z}_k/Z_k$ of the fluctuation field. Contrary to Z_k the square mass m_k^2 enters the flow equation directly. It is the most direct manifestation of the fact that $\Gamma_k[\varphi,\xi]$ is a function of the two variables separately. One could add many other covariant operators to Γ^b_k, but since they would further increase the complexity of the calculations, the following analysis will be restricted to the effects of this simple truncation.

3.3. Beta Functions of the Fourth-Order Derivative Expansion

Having constructed an ansatz for the effective average action one can study the renormalization of the theory by plugging (3.17) into the flow equation (3.14). Projecting the r.h.s. of the flow equation on the operators that appear in the ansatz for Γ_k, it is possible to determine the non-perturbative beta functions of the model. In order to proceed one should define more closely the cutoff kernel appearing in (3.13). A reasonable choice is to coarse-grain the theory relative to the modes of the covariant Laplacian Δ:

$$\mathcal{R}^k_{ab}(\varphi) \quad = \quad Z_k h_{ab} R_k(\Delta)\,. \tag{3.19}$$

The regulator is specified through the non-negative function $R_k(z)$ and is a function of φ solely through the Laplacian. The wave function renormalization of the field ξ^a has been used in (3.19) as an overall parametrization,since the fluctuation field appears quadratic in the cutoff. It is convenient to compute the scale derivative of (3.19) already at this stage. It yields

$$k\partial_k \mathcal{R}^k_{ab}[\varphi] \quad = \quad Z_k h_{ab}\left(k\partial_k R_k(\Delta) - \eta R_k(\Delta)\right)\,. \tag{3.20}$$

For the sake of clarity the beta functions of the two sets of couplings $\{\zeta_k, \alpha_k, L_{1,k}, L_{2,k}\}$ and $\{Z_k, m_k^2\}$ will be computed in two separate steps. The flow of $\Gamma^{\rm s}_k[\phi(\varphi,\xi)]$ can be obtained most easily by considering the limit $\xi \to 0$ of (3.14). The result is a flow equation of the form

$$\begin{aligned} k\partial_k \Gamma^{\rm s}_k[\varphi] \quad &= \quad \frac{1}{2}\mathrm{Tr}\left(\frac{k\partial_k \mathcal{R}_k(\varphi)}{\Gamma^{(0,2)}_k[\varphi,0] + \mathcal{R}_k(\varphi)}\right) \\ &= \quad \frac{1}{2}\mathrm{Tr}\left\{G_k\big(k\partial_k R_k(\Delta) - \eta R_k(\Delta)\big)\right\}, \end{aligned} \tag{3.21}$$

where the modified propagator G_k is the inverse of $Z_k^{-1}{\Gamma_k}^{(0,2)}[\varphi,0] + R_k(\Delta)$. It shows how the fluctuations ξ drive the flow of the couplings $\{\zeta_k, \alpha_k, L_{1,k}, L_{2,k}\}$. The modified propagator is computed from (3.17) using (3.4),(3.11) and (3.18), and reads

$$\begin{aligned} G_k \quad &= \quad \big(P_k(\Delta) + \Sigma\big)^{-1} \\ P_k(\Delta) \quad &= \quad \alpha_k \Delta^2 + \zeta_k \Delta + m^2 \mathbb{1} + R_k(\Delta) \\ \Sigma \quad &= \quad B^{\mu\nu}\nabla_\mu \nabla_\nu + C^\mu \nabla_\mu + D\,. \end{aligned} \tag{3.22}$$

The matrices $B^{\mu\nu}$, C^μ and D are endomorphisms in the tangent space. The explicit form of $B^{\mu\nu}$ and D is

$$\begin{aligned} B^{\mu\nu}_{ab} &= 2\delta^{\mu\nu}(\alpha_k R_{acbd} - T_{abcd})\partial_\rho\phi^c\partial^\rho\phi^d - 4T_{acbd}\partial^\mu\phi^c\partial^\nu\phi^d \\ D_{ab} &= -\zeta_k R_{acbd}\partial_\rho\phi^c\partial^\rho\phi^d - \alpha_k R_{acbd}\Box\phi^c\Box\phi^d \\ &\quad +(\alpha_k R_{acde}R_{bfg}{}^e + 2R_{e(ab)f}T^e{}_{gcd})\partial_\rho\phi^c\partial^\rho\phi^d\partial_\sigma\phi^f\partial^\sigma\phi^g\,. \end{aligned} \tag{3.23}$$

Each term in $B^{\mu\nu}$ and D consists of at least two derivatives of the field φ^a. This implies that a Taylor expansion of (3.22) in Σ is possible, because the chosen truncation ansatz considers only terms up to fourth order in derivatives. The tensor C^μ contains three derivatives of φ^a and thus can be ignored[3]. The possibility to truncate the expansion distinguishes this calculation from the one given in [86], where the operator $\zeta_k\Delta$ was assigned to Σ instead of P_k, such that in principle all orders of the applied heat kernel expansion contribute to the renormalization of the chosen truncation.

The expansion in Σ reads

$$G_k = P_k^{-1} - P_k^{-1}\Sigma P_k^{-1} + P_k^{-1}\Sigma P_k^{-1}\Sigma P_k^{-1} + \mathcal{O}(\partial^6)\,.$$

Inserting this expansion into (3.21) and using the cyclicity of the trace, one obtains

$$k\partial_k\Gamma^{\mathrm{s}}_k[\varphi] = \frac{1}{2}\mathrm{Tr}\, f_1(\Delta) - \frac{1}{2}\mathrm{Tr}\,\Sigma f_2(\Delta) + \frac{1}{2}\mathrm{Tr}\,\Sigma^2 f_3(\Delta) + \mathcal{O}(\partial^6)\,, \tag{3.24}$$

$$\text{with } f_l(z) \equiv \frac{k\partial_k R_k(z) - \eta R_k(z)}{P_k^l(z)}\,. \tag{3.25}$$

The commutator of Σ and $P_k(\Delta)$ in the third term of the expansion was neglected since it is of order $\mathcal{O}(\partial^4)$ and hence will only lead to terms of order $\mathcal{O}(\partial^6)$. The traces appearing in (3.24) can be computed using off-diagonal heat kernel methods [97, 98, 99]. One has to consider the traces

$$\mathrm{Tr}\,\nabla_{\mu_1}\ldots\nabla_{\mu_r} f(\Delta) \tag{3.26}$$

which transform as tensors under isometries and the interest lies in the particular cases $0 \le r \le 4$ and $f(\Delta) = f_l(\Delta)$ for some $l = 1, 2, 3$. Introducing the inverse Laplace transform $\mathcal{L}^{-1}[f](s)$ of $f(z)$, the expression (3.26) can be written as

$$\int_0^\infty ds\,\mathcal{L}^{-1}[f](s)\,\mathrm{Tr}\,\nabla_{\mu_1}\ldots\nabla_{\mu_r}\,\mathrm{e}^{-s\Delta}\,. \tag{3.27}$$

[3] Also the traces linear in ∇_μ do not add up with C^μ to a fourth-order operator but vanish.

The trace $\mathrm{Tr}\,(\nabla_{\mu_1}\ldots\nabla_{\mu_r}e^{-s\Delta})$ is determined by an off-diagonal heat kernel expansion (the case $r=0$ yields the trace of the heat kernel itself). This expansion is an asymptotic small-s expansion that corresponds, for dimensional and covariance reasons, to an expansion in powers of the curvature and covariant derivative. It yields

$$\mathrm{Tr}\,(\nabla_{\mu_1}\ldots\nabla_{\mu_r}e^{-s\Delta}) = \sum_{n=0}^{\infty}\frac{B_{\mu_1\ldots\mu_r,n}}{(4\pi s)^{d/2}}s^{\frac{2n-[r]}{2}}\,, \tag{3.28}$$

where $[r]=r$ if r is even and $[r]=r-1$ if r is odd. The coefficients $B_{\mu_1\ldots\mu_r,n}$ contain a number of powers of the derivatives of the field that increases with n, thus only a finite number of them is needed to compute the traces with $\mathcal{O}(\partial^4)$ accuracy. The relevant elements in the off-diagonal heat kernel expansion of the flow equation (3.24) are

$$\begin{aligned}
\mathrm{Tr}\,e^{s\Delta} &= \frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;\tfrac{1}{12}s^{2-d/2}H_{\mu\nu}H^{\mu\nu} + \text{f.i.c.} + \mathrm{O}(\partial^6)\\
\mathrm{Tr}\,B^{\mu\nu}\nabla_\mu\nabla_\nu e^{s\Delta} &= \frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;\tfrac{1}{2}s^{-d/2}B^{\mu\nu}H_{\mu\nu} - \tfrac{1}{2}s^{-1-d/2}B^{\mu}{}_{\mu} + \mathrm{O}(\partial^6)\\
\mathrm{Tr}\,De^{s\Delta} &= \frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;s^{-d/2}D + \mathrm{O}(\partial^6)\\
\mathrm{Tr}\,B^{\mu\nu}B^{\rho\sigma}\nabla_\mu\nabla_\nu\nabla_\rho\nabla_\sigma e^{s\Delta} &= \frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;s^{-2-d/2}\left(\tfrac{1}{4}B^{\mu}{}_{\mu}B^{\nu}{}_{\nu} + \tfrac{1}{2}B^{(\mu\nu)}B_{\mu\nu}\right) + \mathrm{O}(\partial^6)\\
\mathrm{Tr}\,DB^{\mu\nu}\nabla_\mu\nabla_\nu e^{s\Delta} &= -\frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;\tfrac{1}{2}s^{-1-d/2}DB^{\mu}{}_{\mu} + \mathrm{O}(\partial^6)\\
\mathrm{Tr}\,D^2e^{s\Delta} &= \frac{1}{(4\pi)^{d/2}}\,\mathrm{tr}\int d^dx\;s^{-d/2}D^2 + \mathrm{O}(\partial^6)\,,
\end{aligned} \tag{3.29}$$

where $H_{\mu\nu}$ is the commutator (2.8) of the covariant derivatives evaluated at φ, and "f.i.c." denotes field-independent contributions which only affect the renormalization of the vacuum energy and will hence be neglected.

The final step in computing (3.26) is the s-integration, which can be expressed by *Q-functionals*

$$Q_{n,l} = \frac{1}{(4\pi)^{d/2}}\int_0^\infty ds\, s^{-n}\mathcal{L}^{-1}[f_l](s)\,, \tag{3.30}$$

These equal (for positive n) a Mellin transform[4] of $f_l(z)$:

$$Q_{n,l} = \frac{1}{(4\pi)^{d/2}\Gamma[n]} \int_0^\infty dz\, z^{n-1} f_l(z). \tag{3.31}$$

The running of the effective action is finally given as

$$\begin{aligned} k\partial_k\Gamma^{\mathrm{s}}_k[\varphi] = \frac{1}{2}\mathrm{tr}\int d^dx \Big\{ &\frac{1}{12} Q_{\frac{d}{2}-2,1} H^2_{\mu\nu} + \frac{1}{2}\, Q_{\frac{d}{2}+1,2} B^\mu{}_\mu - \frac{1}{2} Q_{\frac{d}{2},2} B^{\mu\nu} H_{\mu\nu} - Q_{\frac{d}{2},2} D \\ &+ \frac{1}{2} Q_{\frac{d}{2}+2,3} \Big(B^{(\mu\nu)} B_{\mu\nu} + \frac{1}{2} (B^\mu{}_\mu)^2 \Big) - Q_{\frac{d}{2}+1,3} B^\mu{}_\mu D + Q_{\frac{d}{2},3} D^2 \Big\} \end{aligned} \tag{3.32}$$

with the tensors B and D given in (3.23). The beta functions for $\{\zeta_k, \alpha_k, L_{1,k}, L_{2,k}\}$ are denoted by $\{\beta_\zeta, \beta_\alpha, \beta_{L_1}, \beta_{L_2}\}$ and can be extracted by comparing both sides of the flow equation at $\xi = 0$. According to (3.4) the l.h.s. reads

$$\begin{aligned} k\partial_k\Gamma^{\mathrm{s}}_k[\varphi] = \frac{1}{2} \int d^dx\, \Big(&\beta_\zeta \partial_\mu\varphi^a\partial^\mu\varphi_a + \beta_\alpha \Box\varphi^a\Box\varphi_a \\ &+ \beta_{L_1} (\partial_\mu\varphi^a\partial_\nu\varphi_a)^2 + \beta_{L_2} (\partial_\mu\varphi^a\partial^\mu\varphi_a)^2 \Big)\,, \end{aligned} \tag{3.33}$$

and the comparison with the r.h.s. of (3.32) yields the beta functions[5]

$$\begin{aligned} \beta_\zeta =& \zeta(N-2) Q_{\frac{d}{2},2} + \alpha(N-2)d\, Q_{\frac{d}{2}+1,2} - L_1(N+d) Q_{\frac{d}{2}+1,2} - L_2((N-1)d+2) Q_{\frac{d}{2}+1,2} \\ \beta_\alpha =& \alpha\,(N-2)\, Q_{\frac{d}{2},2} \\ \beta_{L_1} =& \frac{1}{6} Q_{\frac{d}{2}-2,1} + \big[(2N-5)L_1 + 2L_2 - \alpha\big] Q_{\frac{d}{2},2} + 2\big[(d+1)L_1 + 2L_2 + d\alpha\big]\zeta Q_{\frac{d}{2}+1,3} \\ &+ \zeta^2 Q_{\frac{d}{2},3} + \Big[(2(N+4) + 4d + d^2)L_1^2 + 8L_2^2 + 4(d+2)L_2\alpha + d(d+2)\alpha^2 \\ &+ 2L_1(2(d+6)L_2 + (d^2+3d+2)\alpha)\Big] Q_{\frac{d}{2}+2,3} \\ \beta_{L_2} =& -\tfrac{1}{6} Q_{\frac{d}{2}-2,1} + \big[L_1 + 2(N-3)L_2 - (N-3)\alpha\big] Q_{\frac{d}{2},2} + (N-3)\zeta^2 Q_{\frac{d}{2},3} \\ &- 2\big[L_2((N-2)d+2) + L_1(N-1+d) - (N-3)d\alpha\big]\,\zeta\, Q_{\frac{d}{2}+1,3} \\ &+ \Big[(d^2(N-1) + 2d(N+1) + 12)L_2^2 + (N+2d+6)L_1^2 + d(d+2)(N-3)\alpha^2 \\ &\quad + 2(d^2+2d+4+N(d+2))L_1L_2 - 2(d+2)(N-1+d)\alpha L_1 \\ &\quad - 2(d+2)(2+d(N-2))\alpha L_2\Big] Q_{\frac{d}{2}+2,3}\,. \end{aligned} \tag{3.34}$$

[4]This reformulation can simply be checked by expressing $f_l(z)$ as a Laplace transform and applying a substitution $zs \to y$, where s is the Laplace parameter. One Q-functional with negative n will appear in the subsequent calculations, which can be computed by the relation $Q_n\big(f(z)\big) = (-1)^i Q_{n+i}\big(\frac{d^i}{dz^i} f(z)\big)$. This can be checked by considering the derivative $\frac{d^i}{dz^i} f(z)$, where $f(z)$ is written as Laplace transform.

[5]suppressing the k subscripts

Finally, the flow of Z_k and m_k^2 has to be determined. The simplest setting for this purpose is a vertex expansion of the flow (3.14) in powers of the field ξ^a. Note that in case of a constant background field φ_c^a the ansatz for the effective action (3.17) reduces to

$$\begin{aligned}\Gamma_k[\varphi_c,\xi] = \frac{Z_k}{2}\int d^dx\Big\{&\zeta_k h_{ab}\nabla_\mu\xi^a\nabla^\mu\xi^b + \alpha_k h_{ab}\Box\xi^a\Box\xi^b + m_k^2 h_{ab}\xi^a\xi^b \\ &+ \frac{1}{3}\zeta_k Z_k R_{abcd}\xi^a\xi^d\nabla_\mu\xi^c\nabla^\mu\xi^b + \frac{4}{3}\alpha_k Z_k R_{abcd}\xi^a\nabla_\mu\xi^b\nabla^\mu\xi^d\Box\xi^c \\ &+ \frac{1}{3}\alpha_k Z_k R_{abcd}\xi^a\Box\xi^b\Box\xi^c\xi^d + Z_k T_{abcd}\nabla_\mu\xi^a\nabla^\mu\xi^b\nabla_\nu\xi^c\nabla^\nu\xi^d\Big\} + \mathcal{O}(\xi^6)\,.\end{aligned} \tag{3.35}$$

In this particular limit the pullback connection (2.7) becomes trivial: $\nabla_\mu = \partial_\mu$ and $\Box = \partial^2$. This observation is particularly useful, as the computations in momentum space become easy. One can define $\xi^a(x) = \int d^dq\, \mathrm{e}^{\mathrm{i}qx}\xi_q^a$ and obtains from (3.35) the 2-point function for incoming momentum p^μ:

$$\Gamma_k^{(0,2)}[\varphi_c,0]_{p,-p} = Z_k(\alpha_k\, p^4 + \zeta_k\, p^2 + m_k^2)\,. \tag{3.36}$$

The target space indices are suppressed in this and the next two equations. The scale derivative reads

$$k\partial_k\Gamma_k^{(0,2)}[\varphi_c,0]_{p,-p} = Z_k\Big((\beta_\alpha - \eta\alpha_k)p^4 + (\beta_\zeta - \eta\zeta_k)p^2 + (\beta_{m^2} - \eta m_k^2)\Big)\,. \tag{3.37}$$

On the other hand, the quantity $k\partial_k\Gamma_k^{(0,2)}[\varphi_c,0]_{p,-p}$ can be computed from (3.14) by applying two functional derivatives w.r.t. ξ^a, taking the limit $\varphi^a = \varphi_c^a = \text{const.}$ and transforming to momentum space. After these manipulations, the flow equation (3.14) reduces to

$$k\partial_k\Gamma_k^{(0,2)}[\varphi_c,0]_{p,-p} = -\frac{1}{2Z_k}\mathrm{Tr}\, f_2(q^2)\Gamma_k^{(0,4)}[\varphi_c,0]_{p,-p,q,-q}\,. \tag{3.38}$$

The momentum space 4-point vertex function $\Gamma_k^{(0,4)}[\varphi_c,0]$ is obtained from (3.35) and is relevant in our computation, while 3-point functions which appear in the derivation vanish for constant φ_c^a. The trace that appears in (3.38) consists of an internal trace on the tangent space of the model, that involves two of the four indices of the 4-vertex, and a momentum space integral $\int d^dq/(2\pi)^d$. The tangent space trace of the 4-point vertex reads

$$\frac{\delta^4\Gamma[\varphi,\xi]}{\delta\xi_{a_1,p}\,\delta\xi_{a_2,-p}\,\delta\xi_{a_3,q}\,\delta\xi_{a_4,-q}}\bigg|_{\substack{\xi=0\\ \varphi_c}} h^{a_3a_4} = -Z_k^2\big[\tfrac{2}{3}\zeta_k(q^2+p^2)+\tfrac{2}{3}\alpha_k p^4+4\alpha_k p^2q^2+\tfrac{2}{3}\alpha_k q^4\big]R_{a_1a_2} + \tfrac{8}{d}Z_k^2q^2p^2T_{a_1\ \ a_2c}^{\ \ c} + 4Z_k^2q^2p^2T_{a_1a_2\ \ c}^{\ \ \ \ \ c} \tag{3.39}$$

The q-integration can be written in terms of Q-functionals and the result is an expression that solely depends on p^2. Comparing the power p^n with $n = 0, 2, 4$ of (3.38) with those of (3.37) and dividing both sides by Z_k, the coefficients can be determined as

$$\begin{aligned}
\beta_\alpha - \eta\alpha_k &= \frac{1}{3}(N-2)\,\alpha_k\,Q_{\frac{d}{2},2}\\
\beta_\zeta - \eta\zeta_k &= \frac{1}{3}(N-2)\zeta_k Q_{\frac{d}{2},2} - \Big((dN-d+2)L_{2,k} + (N+d)L_{1,k} - (N-2)d\alpha_k\Big)Q_{\frac{d}{2}+1,2}\\
\beta_{m^2} - \eta m_k^2 &= \frac{1}{12}(N-2)d(d+2)\,\alpha_k\,Q_{\frac{d}{2}+2,2} + \frac{1}{6}(N-2)d\,\zeta_k\,Q_{\frac{d}{2}+1,2}\,.
\end{aligned} \tag{3.40}$$

As anticipated, there is no explicit dependence on Z_k, as it is a redundant parameter. One interesting feature of the method arises at this point: Using (3.34), one can solve the system of equations (3.40) in terms of the two unknown quantities $\{\eta_k, \beta_{m^2}\}$. For a solution to exist, one equation of (3.40) must be redundant and it is a nontrivial check of our computation, at this stage, that this actually holds true. The final result for the anomalous scaling is

$$\eta_k = \frac{2}{3}\,(N-2)\,Q_{\frac{d}{2},2}\,. \tag{3.41}$$

This section shall be closed with the side note that one could also consider an alternative treatment of the r.h.s. of the flow equation (3.14), which is based on a heat kernel expansion of the Hessian as a fourth-order operator. The first few elements of such an expansion are given in [100]. But this approach is unfeasible, because the coefficients of the heat kernel expansion contain increasing orders of the operator $B^{\mu\nu} + \zeta_k\,\delta^{\mu\nu}$, which means that infinitely many coefficients can in principle contribute to the flow of the considered truncation.

3.4. Phase Diagram in $d = 3$

Having obtained expressions for the beta functions, their structure and the related critical properties ought to be analyzed in more detail. The phase diagram of the two-dimensional case is simple, because it confirms the well-known asymptotic freedom of the theory in two dimensions [41] and hence does not contain a nontrivial fixed point or a phase transition. The focus of this analysis, however, shall lie on the particularly interesting case of three dimensions and the nontrivial critical properties of this model, which have already been studied intensively by other methods, cf. for instance [42, 52, 53].

In order to evaluate the explicit running of the couplings, one first needs to determine explicit expressions for the Q-functionals. This means that a specific regulator (3.19) has to be chosen which fulfills the requirements described in Sec. 2.4. An adapted version of the optimized cutoff (2.34),

$$R_k[z] = \big(\zeta_k(k^2 - z) + \alpha_k(k^4 - z^2)\big)\,\Theta(k^2 - z)\,, \tag{3.42}$$

is a suitable regulator which allows for an explicit calculation of the Q-functionals: (Note that the k-subscript of the couplings will be suppressed in the remainder of this chapter.)

$$Q_{n,l} = \frac{k^{2n+2}}{(4\pi)^{d/2}\,\Gamma(n)}\Big(\frac{(2n+2-\eta+\partial_t)\zeta}{n(n+1)(\zeta k^2+\alpha k^4+m^2)^l} + \frac{2k^2(2n+4-\eta+\partial_t)\alpha}{n(n+2)(\zeta k^2+\alpha k^4+m^2)^l}\Big)\,,$$

The disadvantage of this choice is that the system of differential equations becomes rather involved, since it has to be solved for the derivatives $\partial_t\alpha \equiv k\partial_k\alpha = \beta_\alpha$ and $\partial_t\zeta = \beta_\zeta$, which also appear on the r.h.s. of the flow equation. To study the critical behavior, the canonical dimensions of the couplings ought to be extracted and the equations can be rewritten in terms of dimensionless couplings $\tilde{\zeta} = k^{2-d}\zeta$, $\tilde{\alpha} = k^{4-d}\alpha$, $\tilde{L}_1 = k^{4-d}L_1$ and $\tilde{L}_2 = k^{4-d}L_2$. Plugging the Q-functionals into (3.34) and solving for the scale derivatives it is straightforward to determine the beta functions $\{\beta_{\tilde{\zeta}}, \beta_{\tilde{\alpha}}, \beta_{\tilde{L}_1}, \beta_{\tilde{L}_2}\}$, which are involved rational functions and hence not given here explicitly.

Now everything is prepared to study the phase diagrams and the critical properties which arise from these flow equations. It is instructive to proceed in a systematic way, by considering step-by-step more and more operators of the truncation. The simplest truncation which only contains the coupling ζ was already studied in [43]. The computations outlined above confirm the results of this investigation and find a nontrivial fixed point at $\tilde{\zeta}^* = 16(N-2)/(45\pi^2)$. The N-dependence of the critical exponent ν and its relation to the eigenvalues of the stability matrix were already described in Sec. 2.4. While the critical value $\tilde{\zeta}^*$ depends linearly on N, the critical exponent $\nu^{-1} = \Theta^R = -\frac{d}{d\tilde{\zeta}}\beta_{\tilde{\zeta}}|_{\tilde{\zeta}^*}$ is independent of N: it is 16/15 for all N. In this sense the computation is a reminiscent of the one-loop large-N calculations [51], apart from the small deviation of the critical exponent from the large-N value 1. In order to become sensitive to this N-dependence, one apparently has to include higher order operators. This agrees with the argument given in Sec. 3.1 that the beta functions for different homogenous spaces have the same structure if one considers a simple truncation [43]. In order to distinguish between the models and to become sensitive to their specific properties, further operators have to be taken into account. Following this idea, the coupling α and the related fourth-order operator can be included. The corresponding renormalization group flow is depicted in Fig. 3.1 and confirms the nontrivial fixed point found in the simpler truncation. The case $N = 3$ is presented as an example, while the flow diagrams for larger N differ from Fig. 3.1 only in the N-dependent position of the fixed point which is situated at $\tilde{\zeta}^* = 16(N-2)/(45\,\pi^2)$ and $\tilde{\alpha}^* = 0$. Since α is apparently not generated in this truncation, the system of two couplings effectively reduces to the one-parameter truncation just discussed.

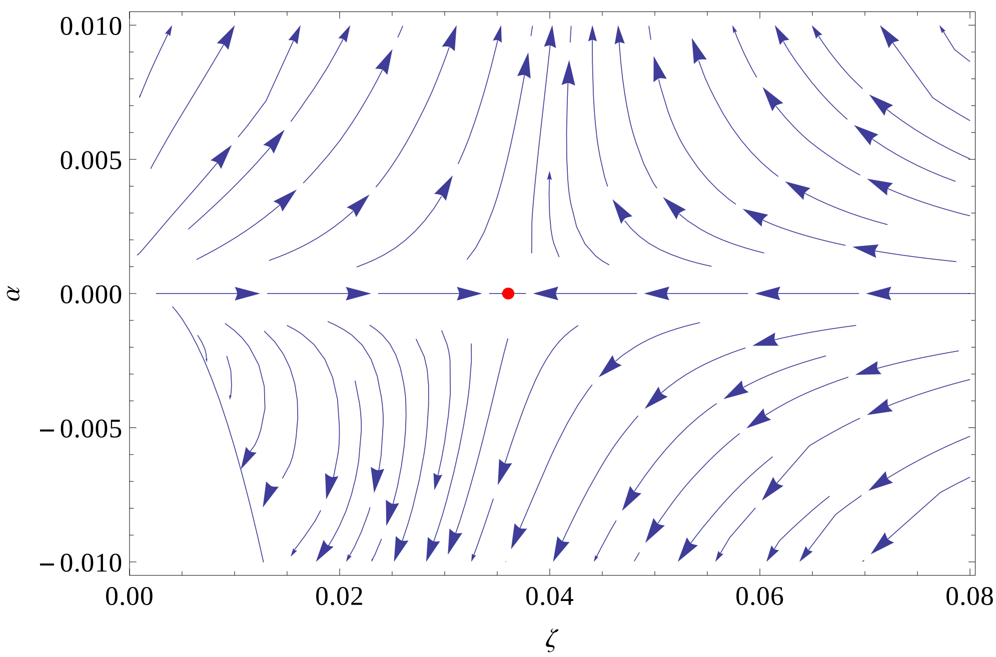

Figure 3.1.: The flow of the couplings $\tilde{\zeta}$ and $\tilde{\alpha}$ calculated for $N=3$ in the truncation $\{\zeta, \alpha\}$. The arrows point toward the ultraviolet. The removed region lies beyond an unphysical singularity which is introduced by the choice of the cutoff.

Note that the arrows of the flow point into the direction of increasing k, i.e. towards the ultraviolet. It is interesting to note that the coupling α belongs to an IR-irrelevant operator and exactly vanishes at the fixed point. In fact, already the simple structure of β_α which is given in (3.34) reveals that α has to vanish for every possible fixed point, as the flow of the dimensionless coupling $\tilde{\alpha}$ reads in $d = 3$:

$$\beta_{\tilde{\alpha}} = \tilde{\alpha} + (N-2)\, Q_{\frac{3}{2},2}\, \tilde{\alpha} \tag{3.43}$$

Since $Q_{\frac{3}{2},2}$ is strictly positive for any reasonable regulator, see (3.31), the only possible fixed point value is $\tilde{\alpha} = 0$. This statement remains true when the couplings L_1, L_2 are included. There is also a fixed point for $\lambda = 1/\alpha = 0$, but this is a trivial one whose critical exponents are equal to the canonical mass dimensions of the operators. It is the three-dimensional analogue of the fixed point in four dimensions which is discussed in [86].
The result $\tilde{\alpha}^* = 0$ agrees with an alternative computation of the effective action of the nonlinear O(N) model up to fourth order, which is presented in [54], and in which a term $\propto \partial^2\phi\partial^2\phi$ is not generated, either. However, it is very likely that an extension of the truncation to the sixth order in derivatives and an inclusion of operators like e.g. $\Box\phi_a\Box\phi^a\partial_\mu\phi^b\partial^\mu\phi_b$ will affect the running of α and shift the position of the fixed point.
In a next step, the truncation can be extended by adding $L_1(h_{ab}\partial_\mu\phi^a\partial_\nu\phi^b)^2$. The resulting flow of the couplings $\tilde{\zeta}$ and $\tilde{L}_1$ of the O(3) model is depicted in Figure 3.2, where the irrelevant coupling $\tilde{\alpha}$ is set to $\tilde{\alpha}^* = 0$. It contains the nontrivial fixed point which was already discovered in the leading order truncation and which has only one relevant direction. The fixed point exists for all N, and while the critical value of $\tilde{L}_1$ is almost independent of N and close to -0.013, the fixed point value $\tilde{\zeta}^*$ is an involved expression in N which for $N = 3$ attains the values 0.059. It increases with N and approaches a linear function with a slope of roughly 0.036 for large N. There are actually additional fixed points in the truncation with couplings ζ, α and L_1, some with negative $\tilde{\zeta}^*$ and one with quite large values of $\tilde{L}_1^*$ and $\tilde{\zeta}^*$. These could be artifacts of the choice (3.42) of the cutoff functions which may develop singularities for negative couplings. It does not seem to be possible to relate the additional fixed points to known critical properties of sigma models and their physical relevance remains doubtful. The focus of these investigation will hence lie on the fixed point depicted in Figs. 3.1 and 3.2.
As anticipated, the inclusion of a non-vanishing fourth-order operator renders the exponent ν sensitive to the dimension of the target space. The N-dependence of the exponent is depicted in Fig. 3.3, while the numerical values are given in Tab. 3.1.
Since $\nu(N)$ is a very involved and long expression, it is more instructive to study selected values of N. The values in the third row denoted by “full system” refer to calculations with the truncation $\{\zeta, \alpha, L_1\}$, in which the anomalous scaling η of the fluctuation fields ξ is taken into account. If one sets $Z \equiv 1$, one obtains the

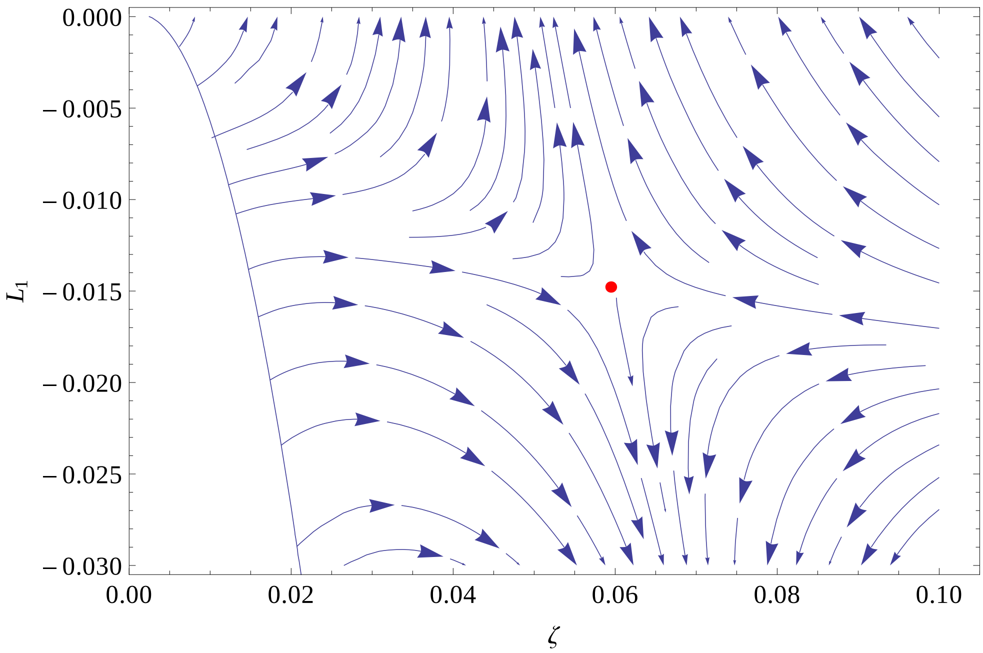

Figure 3.2.: The flow of the couplings $\tilde{\zeta}$ and $\tilde{L}_1$ towards the UV for $N = 3$. It was calculated in the truncation $\{\zeta, \alpha, L_1\}$ and depicts the plane $\tilde{\alpha} = \tilde{\alpha}^* = 0$. The fixed point is at $\tilde{\zeta}^* = 0.059$ and $\tilde{L}_1^* = -0.013$ and has one IR-relevant direction.

N	3	4	6	8	10	20
adiabatic approx.	0.824	0.924	0.969	0.981	0.987	0.995
with $Z = 1$	0.654	0.756	0.802	0.815	0.820	0.828
full system	0.704	0.833	0.895	0.912	0.920	0.931
literature	0.710	0.747	0.790	0.830	0.863	0.934

Table 3.1.: The critical exponent ν for various values of N and different approximations. The last row contains the best-known values from the literature.

values in the second row of Table 3.1. If one neglects, in addition, the k-derivative of the couplings in $k\partial_k\mathcal{R}_k$ on the r.h.s. of the flow equation, that amounts to an adiabatic approximation, then one obtains the values in the first row of Table 3.1. At the fixed point the k-derivative of the couplings vanish such that the approximation with $Z = 1$ and the cruder adiabatic approximation yield the same fixed point couplings.

The last row serves for a comparison with values taken from the vast literature about the critical properties of the O(N) universality class. For $N = 3$ and $N = 4$ the values are taken from the review [42], which contains the results of many independent computations of which the non-biased mean values were taken. For $N > 5$ the mean values of the results in [53, 80, 81] were used, which have been obtained by a high-temperature expansion, a strong-coupling expansion and six-loop RG expansion including a Padé-Borel resummation. The corresponding values deviate from each other by less than two percent.

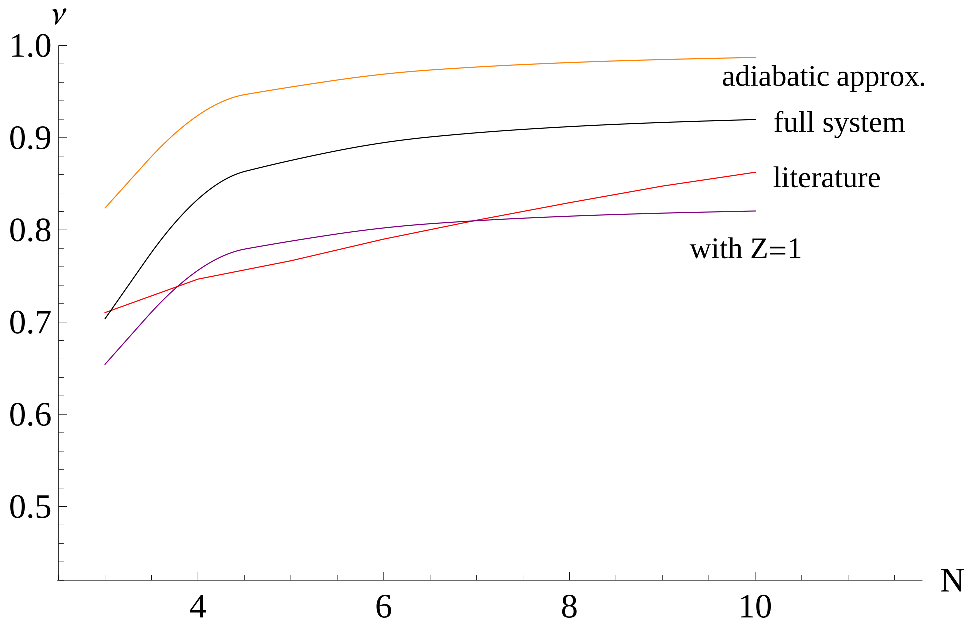

Figure 3.3.: The critical exponent ν as function of N, computed in the truncation $\{\zeta, \alpha, L_1\}$. Depicted are the results of various approximations in comparison with average values from the literature.

The three variations of the calculation which are presented here yield a critical exponent ν whose N-dependence roughly agrees with the results in the literature. The values obtained in the adiabatic approximation deviate considerably from the references values for small N, but show the correct large-N asymptotic $\lim_{N\to\infty} \nu = 1$. If one takes the running of the couplings in $k\partial_k \mathcal{R}_k$ into account, the results for small N improve significantly, especially if one neglects the wave function renormalization. For large N, however, $\nu(N)$ approaches the value $5/6$ instead of 1. If one includes the wave function renormalization, one obtains a critical exponent $\nu(N)$ which is closer to the reference value than the adiabatic result and whose asymptotic behavior is better behaved as in the approximation with $Z = 1$. The deviation from the best-known value is maximal for $N = 5$, where it is 14%, and the asymptotic value is $15/16$ instead of 1. This is in fact the value that was found in the reduced truncation with just one coupling and this agreement originates from $\lim_{N\to\infty}(\tilde{L}_1^*/\tilde{\zeta}^*) = 0$.
The wave function renormalization was included mainly for conceptual reasons, because the background and fluctuation fields are treated differently in the FRG formalism and hence may possess different renormalization properties. It is not clear to

what extent the scaling parameter Z improves the situation: on one hand a running Z improves $\nu(N)$ for large N, while on the other hand $Z = 1$ yields more accurate results for small N.
Also the mass parameter m_k^2 was included in order to examine if terms that go beyond the ansatz of a single-field functional can improve the accuracy of the results. A truncation with couplings $\{\zeta, \alpha, L_1, m^2\}$ leads to the same fixed point as before with slightly modified critical values and a positive mass parameter. However, the results for the critical exponent get worse rather than better and are even a bit worse than the values of the adiabatic approximation, yielding an asymptotic value for ν of roughly 1.146. This is a surprising finding and certainly requires a better understanding. For this purpose, the effects of higher-order terms in $\Gamma_k^b[\varphi, \xi]$ have to be studied.
Finally, the remaining operator with four derivatives, $L_2(h_{ab}\partial_\mu\phi^a\partial^\mu\phi^b)^2$, ought to be included. Although it is of the same order as the operators with couplings L_1 and α, it changes the flow more significantly, such that there is no nontrivial fixed point for the system with couplings $\{\zeta, \alpha, L_1, L_2\}$. This statement holds true for all possible modifications of the flow, i.e. in the adiabatic approximation, in the approximation with $Z = 1$ and also if one includes a mass parameter. In fact, already in the cruder truncation $\{\zeta, \alpha, L_2\}$ there is no nontrivial fixed point and it seems as if the renormalization of the coupling L_2 is not well-balanced. The destabilization of the flow induced by the L_2-term does not seem to depend on a specific choice of regulator. The alternative regulator $R_k(z) = k^{d+2}/z$ was explicitly tested and it confirmed the existence of nontrivial fixed points as well as the N-dependence of ν in the truncation $\{\zeta, \alpha, L_1\}$, but also the disappearance of the fixed point if one includes L_2.
One may wonder why this term with four derivatives destabilizes the renormalization group flow. In the computation of the full effective action, the renormalization of an operator of a given order is always affected by operators of higher orders. These contributions are lost if one applies a truncation. In the present case the beta functions of L_1 and L_2 are quadratic functions in the couplings, see (3.34), and the coefficients of the polynomials must be fine tuned such that both beta functions vanish. In fact, the beta function of L_2 is nearly zero, when evaluated at the fixed point for the subsystem consisting of all other couplings. It is a reasonable expectation that the inclusion of higher order terms will slightly modify the flow in a way that one can recover the fixed point and the information about the phase transition of the O(N) model, that already show up in the truncation $\{\zeta, \alpha, L_1\}$.
However, there could be more subtle explanations why the flow of the operator

$(h_{ab}\partial_\mu\phi^a\partial^\mu\phi^b)^2$ does not lead to a stable fixed point. Only two possibilities shall be mentioned: In order to find a stable fixed point for the full system, one has to enlarge the truncation consistently with regard to hidden symmetries involving the background and the fluctuation fields. To this day the background field method is the most effective way to deal with nontrivial field-space geometries in the framework of the FRG. Nevertheless, further studies maybe needed to understand better which truncations in terms of background and fluctuation fields ought to be chosen in order to maintain the full reparametrization invariance of the theory. An ansatz that is based on the so-called Nielsen identities was presented recently in the context of gravity [95] and it could be interesting to apply this approach to the nonlinear sigma model, too.
The second possibility is related to the arguments brought forward in [22] that the regularization procedure of the FRG based on ΔS_k may require a corresponding modification of the path integral measure, which in turn leads to an additional term in the flow equation of the effective average action. While this term yields only a renormalization of the vacuum energy in theories with linearly realized symmetries, it can affect the renormalization of nontrivial operators in nonlinear theories. Possible consequences for the calculations presented above will be discussed in Sec. 4.1.

3.5. Monte Carlo Renormalization Group

While the FRG naturally addresses the renormalization properties of physical theories, the starting point of Monte Carlo studies is the measurement of observables as expectation values computed on large sets of field configurations. The running of a coupling has to be determined by indirect methods that modify the UV cutoff which in numerical simulations is naturally given by the lattice spacing a, $\Lambda = \frac{\pi}{a}$. Fluctuations above this scale cannot be resolved and are implicitly taken into account in the definition of the lattice action as an effective action at $k = \Lambda$. The IR cutoff is naturally set by the extent of the lattice, $\lambda = \frac{\pi}{L} = \frac{\pi}{N_L a}$. The investigations in this section are performed on three-dimensional lattices with equal temporal and spatial extent $N_L = N_T$, i.e. at zero temperature. The physical volume is hence $V = L^3 = (N_L a)^3$.
The idea of the Monte Carlo Renormalization Group (MCRG) is to combine the efficient numerical tool of Monte Carlo simulations with RG transformations based on the initial idea of block spins [63]. After it was first suggested in [101], it was developed in different directions [102, 103], which for instance employ a direct matching

of simulations at different lattices sizes. Since such procedures usually become very expensive quickly, an alternative approach of MCRG will be used here instead, which employs a microcanonical *demon method* [104]. It shall be briefly described here: First, field configurations $\{\boldsymbol{n}_x\}$ are generated on a lattice (N_L, a) by a Monte Carlo algorithm from a lattice action with couplings $\{g_i\}$. Based on these, new configurations $\{\boldsymbol{n}'_x\}$ on a smaller lattice (N'_L, a') are determined by a block spin transformation as averages of 2^3 hypercubes on the initial lattice. These coarse-grained configurations $\{\boldsymbol{n}'_x\}$ could have been generated also from a certain action on the lattice (N'_L, a'), given by a set of couplings $\{g'_i\}$. This set will contain in most cases an infinite number of effective couplings, but for practical purposes one has to restrict the analysis, like in FRG computations, to a finite ansatz

$$S[\boldsymbol{n}] = \sum_{i=1}^{s} g'_i \, S_i[\boldsymbol{n}] \,, \tag{3.44}$$

and one assumes that the distribution of the states can be described sufficiently well by the weight corresponding to this truncated action. Now a *demon* system is considered, which is defined by the action

$$S^D = \sum_{i=1}^{s} g'_i \, E_i^D \,, \tag{3.45}$$

where the E_i^D are just real numbers taking values in some given range $(-E_m, E_m)$. If one couples both systems, the joint canonical partition sum reads

$$\mathcal{Z}_{Can} = \int_{-E_m}^{E_m} \prod_i dE_i^D \int_\Gamma \mathrm{e}^{-\sum\limits_{i=1}^{s} g'_i \, (S_i + E_i^D)} \,, \tag{3.46}$$

where Γ denotes the configuration space. The expectation values $\left\langle E_i^D \right\rangle_{Can}$ of the demon energies can be computed exactly, since the integral factorizes and E_i^D is constrained:

$$\left\langle E_i^D \right\rangle_{Can} = \frac{1}{g'_i} - \frac{E_m}{\tanh(g'_i E_m)} \,. \tag{3.47}$$

This equation provides an invertible relation between g'_i and $\left\langle E_i^D \right\rangle_C$. Assuming that the lattices are large enough, the expectation value of the canonical ensemble can be approximated by the microcanonical one. This expectation value, however, can be computed without explicit reference to the coupling g'_i by a microcanonical Monte

Carlo simulation in accordance with

$$\left\langle E_j^D \right\rangle_{Mic} = \frac{1}{\mathcal{Z}_{Mic}} \int_{-E_m}^{E_m} \prod_i dE_i^D \int_\Gamma \; E_j^D \, \delta(S_i + E_i^D - S_i^0) \,, \tag{3.48}$$

$$\text{with } \mathcal{Z}_{Mic} = \int_{-E_m}^{E_m} \prod_i dE_i^D \int_\Gamma \; \delta(S_i + E_i^D - S_i^0) \,. \tag{3.49}$$

The simulation starts at some configuration (for which the operators S_i assume the values S_i^0) and generates by a standard update algorithm new configurations, for which the operators will assume some new values S_i' and which are accepted if $S_i' - S_i^0 \in (-E_m, E_m)$. By an iteration of such generation and acceptance steps sufficiently many elements of the partition sum $\mathcal{Z}_{Mic}$ can be determined, on which $\left\langle E_i^D \right\rangle$ can be measured as average values. With these expressions for the expectation values, one can directly obtain $\{g_i'\}$ from (3.47). Note that in order to reduce the dependence on the specific starting configuration, an improvement was suggested in [105] which employs a set of statistically independent starting configurations.

Knowing $\{g_i\}$ and $\{g_i'\}$ one can immediately determine the beta functions. While the physical volumne remains unchanged under the block spin transformations (i.e. the IR cutoff is not affected), the lattice spacing is doubled by an averaging over 2^3 hypercubes and the UV cutoff is hence halved:

$$N_L' = \frac{N_L}{2} \,, \quad a' = 2a \Rightarrow \Lambda' = \frac{\Lambda}{2}. \tag{3.50}$$

The running of the couplings is then given as

$$\beta_{g_i} = -a \frac{\partial g_i}{\partial a} = -(g_i' - g_i) \,. \tag{3.51}$$

So far the block spin transformation was described as a simple averaging over a hypercube of the initial lattice. However, it was shown in [106] that an improved block spin transformation is in fact more efficient in MCRG studies. In this improved transformation the configurations $\{\boldsymbol{n}_x'\}$ are statistically generated according to the normalized probability distribution

$$\frac{1}{\mathcal{N}} \exp\big(c(g_i)\, \boldsymbol{n}_x' \cdot R(\boldsymbol{n})\big) \,, \tag{3.52}$$

where $R(\boldsymbol{n}) = \sum_{y \in \Box} \boldsymbol{n}_y$ is the sum over the configuration values in some 2^3 hypercube $\Box$ of the (N_L, a) lattice. The outlined procedure assignes to hypercubes in the initial configuration an unique field value $\boldsymbol{n}_x'$ on the coarse-grained lattice. The parameter $c(g_i)$ determines how strongly $\boldsymbol{n}_x'$ may fluctuate around the mean value of the underlying degrees of freedom. Although an arbitrarily large $c(g_i)$ would ensure a strict alignment, some smoothening is deliberatly taken into account, because it shifts the system closer to the renormalized trajectory [106] and thus reduces the error which is made by truncating the action. This shift and hence the improvement depends on the position in coupling space. In order to find an appropriate parameter $c(g_i)$, an ansatz in the couplings should be chosen and the coefficients should be fine tuned such that measurements of physical observables on the initial lattices, like e.g. the masses, agree with the computation of these observables on the coarse-grained lattices with couplings $\{g_i'\}$.

A comparison of the MCRG technique with the FRG calculations performed in the previous section requires a truncation (3.44) which corresponds to (3.4) and includes all operators up to fourth order in the derivatives. Note that an implementation of the purely bosonic nonlinear O(N) models is particularly efficient in terms of explicitly constrained fields, which enable to use the elements of SO(N) as dynamical variables by writting each field as $\boldsymbol{n}_x = O_x \boldsymbol{n}_0$ with $O_x \in \mathrm{SO}(N)$. The ansatz for the action functional is therefore chosen as

$$S[\boldsymbol{n}] = \sum_{i=1}^{4} g_i \, S_i[\boldsymbol{n}] + \mathcal{O}(\partial^6) \tag{3.53}$$

where n^a are constrained N-tuple with $\boldsymbol{n}^2 = 1$ and the continuum operators read

$$S_1 = \int d^3x \, \partial_\mu \boldsymbol{n} \partial^\mu \boldsymbol{n} \, , \qquad S_2 = \int d^3x \, \partial^2 \boldsymbol{n} \partial^2 \boldsymbol{n} \, , \tag{3.54}$$

$$S_3 = \int d^3x \, (\partial_\mu \boldsymbol{n} \partial_\nu \boldsymbol{n})(\partial^\mu \boldsymbol{n} \partial^\nu \boldsymbol{n}) \, , \qquad S_4 = \int d^3x \, (\partial_\mu \boldsymbol{n} \partial^\mu \boldsymbol{n})^2 \, . \tag{3.55}$$

There is no direct one-to-one-correspondence between the operators in (3.53) and (3.4), but the relation between both expansions can be derived easily by a suitable change of coordinates, as it is depicted in appendix A.1. It yields

$$\begin{aligned}\mathcal{L}_{\mathrm{eff}} =& \tfrac{1}{2} \, \zeta \, h_{ab} \partial_\mu \phi^a \partial^\mu \phi^b + \tfrac{1}{2} \, \alpha \, h_{ab} \Box \phi^a \Box \phi^b + \tfrac{1}{2} \, L_1 (h_{ab} \partial_\mu \phi^a \partial_\nu \phi^b)^2 + \tfrac{1}{2} \, L_2 (h_{ab} \partial_\mu \phi^a \partial^\mu \phi^b)^2 \\ =& \tfrac{1}{2} \, \frac{\zeta}{4} \, \partial_\mu \boldsymbol{n} \partial^\mu \boldsymbol{n} + \tfrac{1}{2} \, \frac{\alpha}{4} \, \partial^2 \boldsymbol{n} \partial^2 \boldsymbol{n} + \tfrac{1}{2} \, \frac{L_1}{16} \, (\partial_\mu \boldsymbol{n} \partial_\nu \boldsymbol{n})^2 + \tfrac{1}{2} \, \frac{L_2 - 4\alpha}{16} \, (\partial_\mu \boldsymbol{n} \partial^\mu \boldsymbol{n})^2 \, .\end{aligned} \tag{3.56}$$

It should be stressed that, although the two truncations (3.53) and (3.4) span the same subspace in operator space, the truncation procedure works differently in FRG and MCRG calculations. While operators of higher orders are completely neglected in computations of the FRG, Monte Carlo simulations incorporate all possible operators that are generated and the configurations $\{\boldsymbol{n}_x\}$ are thus affected by these. The demon methods determines the renormalization of the chosen truncation based on these configurations and hence takes also the influence of the higher-order operators into account. Keeping this in mind one can turn towards the explicit analysis of the renormalization flow.

Since the implementation and the execution of the Monte Carlo RG algorithm were performed by Daniel Körner and Björn Wellegehausen, only some first results shall be briefly depicted in this thesis with a particular emphasis on the comparison with the FRG computations presented in the previous section. Note that these results are preliminary and focussed on the case $N = 3$. An extended discussion based on conclusive results is supposed to appear soon [107], including a more detailed description of the implementation.

The continuum operators are discretized by the replacement rules

$$\partial_\mu \boldsymbol{n}(x) \to \boldsymbol{n}_{x+\hat{\mu}} - \boldsymbol{n}_x \quad \text{and} \quad \partial^\mu \boldsymbol{n}(x) \to \boldsymbol{n}_x - \boldsymbol{n}_{x-\hat{\mu}}, \tag{3.57}$$

where the lattice spacing $a = 1$ was assumed and $\hat{\mu}$ denotes the unit vector in direction μ. As an example, the first two terms of the truncation read:

$$S_1 = 2\sum_{x,\mu} \boldsymbol{n}_x \cdot \boldsymbol{n}_{x+\hat{\mu}} - 6V \tag{3.58}$$

$$S_2 = 2\sum_{x,\mu,\nu} \boldsymbol{n}_x \cdot (\boldsymbol{n}_{x+\hat{\mu}+\hat{\nu}} + \boldsymbol{n}_{x+\hat{\mu}-\hat{\nu}}) - 12\sum_{x,\mu} \boldsymbol{n}_x \cdot \boldsymbol{n}_{x+\hat{\mu}} + 36V \tag{3.59}$$

The discretized form of S_1 apparently appears as a term in the discretized operator S_2. In order to avoid mixing between the lattice operators, especially in the demon method, the action functional is rewritten, such that the computation for the two-coupling truncation, for instance, are in fact performed for the ansatz

$$S = G_1\,\tilde{S}_1 + G_2\,\tilde{S}_2\,, \tag{3.60}$$
$$\text{with } G_1 = g_1 - 6g_2,\ G_2 = g_2,\ \text{and } \tilde{S}_1 = S_1,\ \tilde{S}_2 = 2\sum_{x,\mu,\nu} \boldsymbol{n}_x \cdot (\boldsymbol{n}_{x+\hat{\mu}+\hat{\nu}} + \boldsymbol{n}_{x+\hat{\mu}-\hat{\nu}})\ .$$

A similar rearrangement, introducing G_3 and G_4, is applied, if one takes the further operators into account. While this reformulation is necessary to improve the algorithm, it makes the comparison to the FRG flows more difficult.

Following to the outlined procedure, the renormalization of the fouth-order expansion (3.53) was investigated by block spin transformations from 32^3 to 16^3 lattices. A linear ansatz in G_1 and G_2 was chosen for the transformation parameter $c(G_i)$ and

test simulations with a focus on the measurement of the physical mass suggested to choose $c(G_i) = 3.4\,G_1 + 0.6\,G_2$.
Analogous to Sec. 3.4 the truncation can be extended step by step, beginning with the simple truncation $\{G_1, G_2\}$. For two couplings it is still feasible to compute at each point $\{G_i\}$ on a certain array in parameter space the corresponding $\{G_i'\}$. The resulting flow diagram for the case $N = 3$ is displayed in Fig. 3.4, with the arrows of the flow pointing towards the IR.

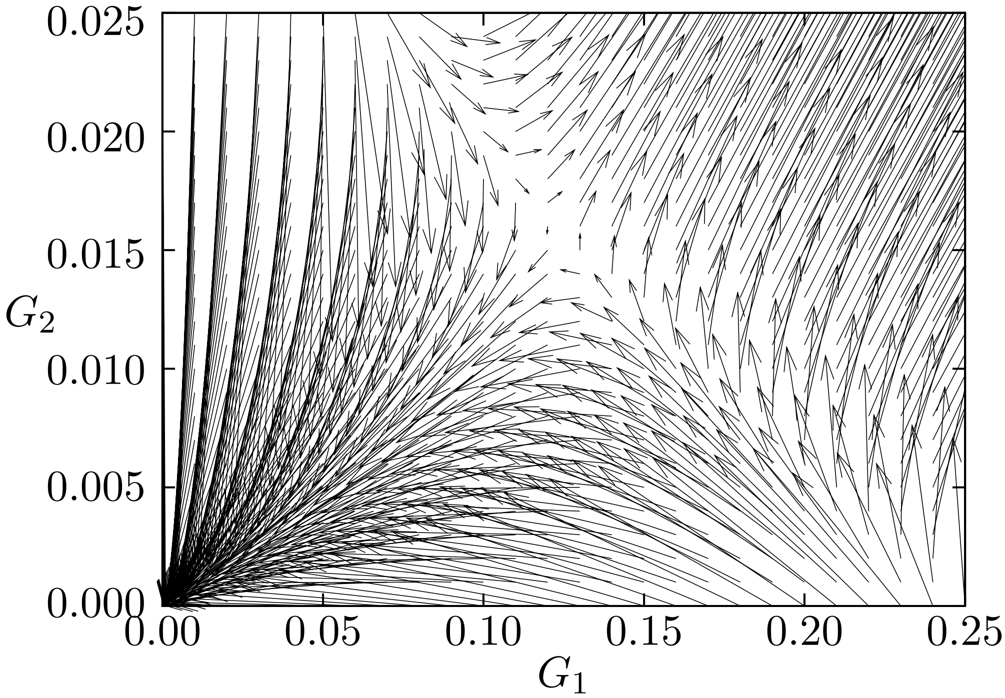

Figure 3.4.: The renormalization flow for the truncation with two couplings G_1 and G_2 for $N = 3$. The arrows point towards the infrared.

In accordance with the results of the FRG computations, a nontrivial fixed point can be identified clearly, which has one IR-relevant and one IR-irrelevant direction and is situated at approx. $(G_1^* = 0.122, G_2^* = 0.0158) \cong (g_1^* = 0.217, g_2^* = 0.0158)$. The position of the fixed point does not agree with the findings of the FRG, as a vanishing α^* corresponds according to (3.56) to a vanishing g_2^*. This deviation, however, is not surprising, since the exact position of the fixed point always depends on the regularization scheme. Furthermore, it was already emphasized that the MCRG computations are sensitive to generated operators of higher orders which affect the value of α^*, and one can assume that an extension of the FRG truncation would also lead to a non-vanishing α^*. While an exact quantitative agreement cannot be expected, the structures of the renormalization flows Fig. 3.4 and Fig. 3.1 match and show qualitative agreement between the two different methods.

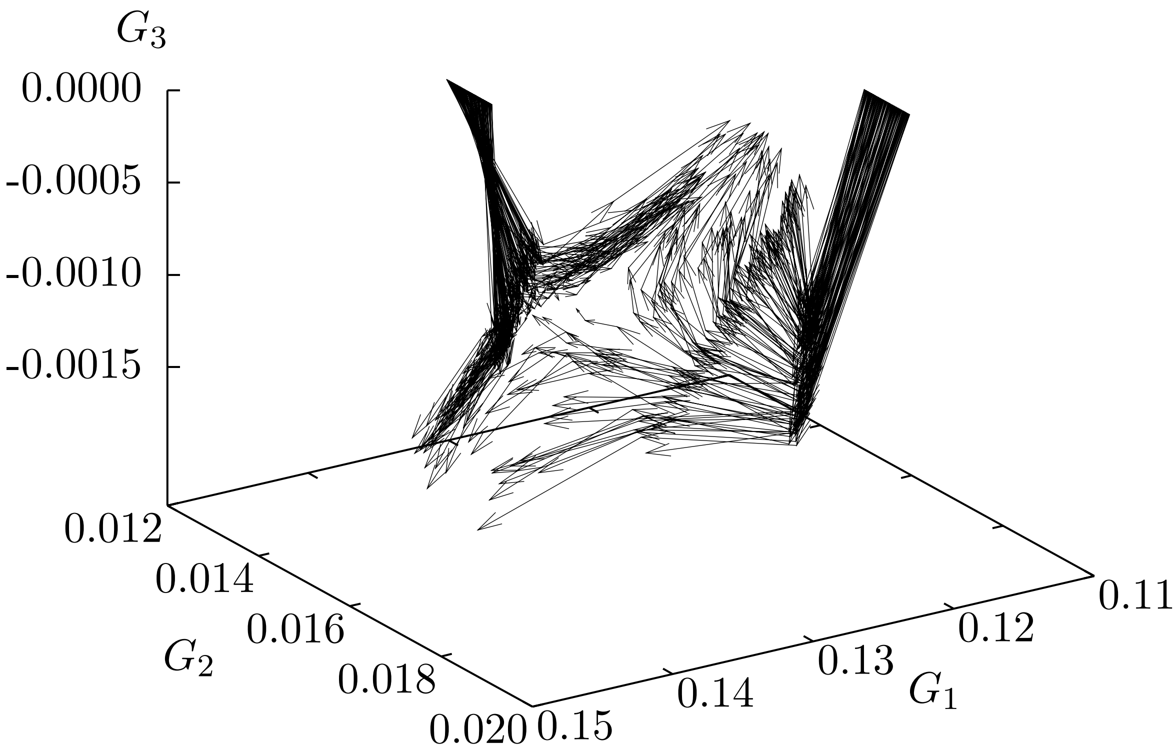

Figure 3.5.: The renormalization flow towards the IR for $N = 3$ computed in the full fourth-order truncation, projected on the subspace $\{G_1, G_2, G_3\}$.

Because the rearrangement of the MCRG couplings prevents a direct comparison of truncations with three couplings, one can directly include G_3 and G_4 in a next step and study the qualitative features of the full fourth-order renormalization flow. The result for $N = 3$ is given in Fig. 3.5 and Fig. 3.6, in which the four-dimensional flow is projected for the sake of presentation on the subspaces $\{G_1, G_2, G_3\}$ and $\{G_1, G_2, G_4\}$. A systematic computation of the flow on an array in parameter space becomes inefficient in the enlarged parameter space. Instead, some trajectories are explicitly determined by using renormalized couplings on the 16^3 lattice as initial values on the 32^3 lattice in a subsequent block spin transformation.

The computations confirm the nontrivial fixed point which was already present in the reduced truncation. Similar to the finding in the $\{\zeta, \alpha, L_1\}$ truncation of the FRG analysis, the fourth-order operators only add irrelevant directions to the parameter space. Furthermore, the critical values of the higher order couplings are in both calculations much smaller than the dominant first-order coupling ζ or G_1. In contrast to the FRG computations, however, the MCRG flow and its fixed point remain stable even if one includes all fourth-order operators. This finding supports the conclusion of the FRG studies that the missing fixed point in the full fourth-order system is only the result of an unbalanced truncation which probably will be stabilized if one includes the effects of higher-order operators (to which the MCRG computations are already sensitive). Being a complementary tool to investigate non-perturbative effects, the numerical simulations on the lattice are able to provide further evidence for the non-perturbative renormalizability of the model and hence for the asymptotic safety scenario.

Note that, although the focus of the MCRG computation was so far on the O(3) model, test computations were performed for larger N which indicate similar but shifted structures as for $N = 3$. Furthermore, if one systematically computes the discrete beta functions on an array in parameter space, it is straightforward to calculate the stability matrix as differences of these beta functions at neighouring array points. Both issues are addressed by further numerical studies which will be presented, together with additional results concerning the discussion above, in an upcoming article [107].

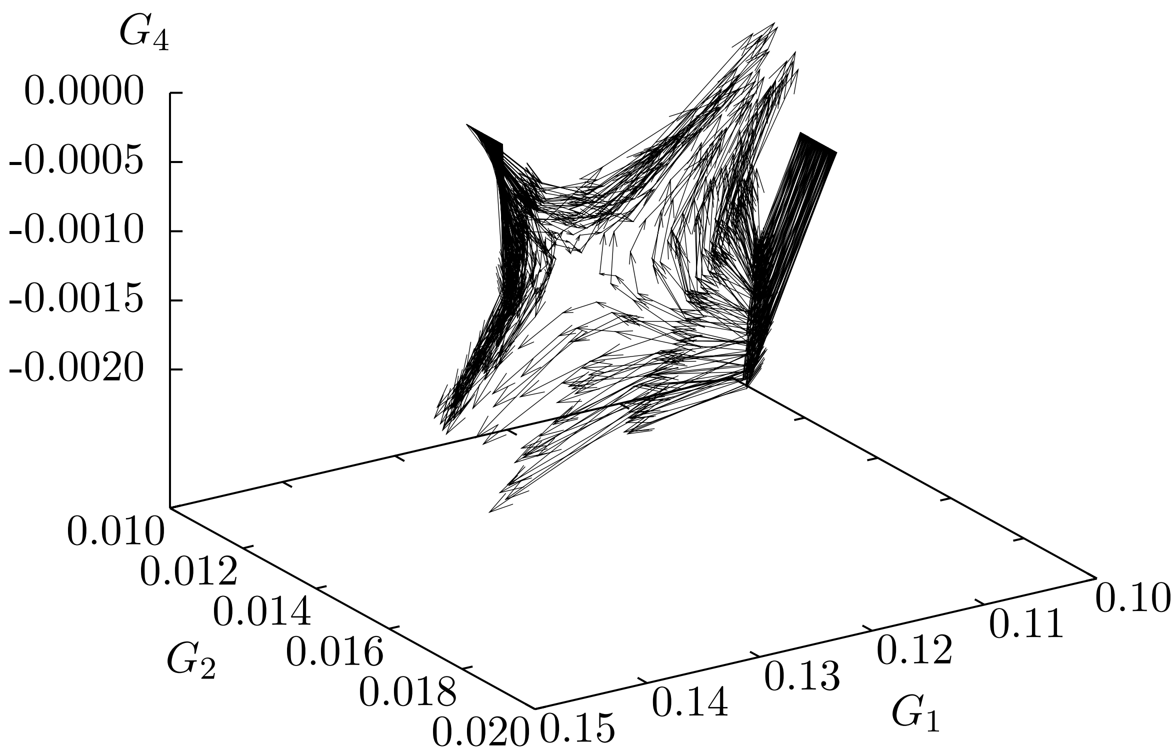

Figure 3.6.: The renormalization flow towards the IR for $N = 3$ computed in the full fourth-order truncation, projected on the subspace $\{G_1, G_2, G_4\}$.

3.6. Conclusions

The renormalization properties of nonlinear O(N) models were investigated by means of the analytic FRG and the numerical MCRG. Although the conceptual aspects and derivations apply for general dimensions, the focus of the discussion was on $d = 3$, since this case is interesting with regard to the concept of non-perturbative renormalizability, is still efficiently accessible by numerical simulations and provides well-studied critical properties which can serve as benchmarks.
Starting with the FRG approach the nonlinear models were studied first as the limit of linear ones. However, all information that is accessible in this way (by a reasonable amount of computational effort) only corresponds to a simple truncation in a nonlinear formulation and is not sensitive to the nontrivial critical properties of the model.
Therefore, a manifestly nonlinear analysis of the model was developed instead and applied to a truncation which includes all covariant operators up to fourth order in derivatives. The flow equation was formulated in a manifestly reparametrization invariant way, so that the results do neither depend on any specific choice of coordinates on the target sphere, nor on an implicit embedding of the model into a linear space. Since the symmetries of the theory are realized nonlinearly, a geometric formulation was adopted in which a background (base point) dependence is introduced in order to maintain the covariance of the model. Moreover, the background field was used to construct a quadratic infrared cutoff term for the fluctuations, whose purpose is to allow for an effective integration of the ultraviolet modes while simultaneously respecting the symmetries of the model. The resulting scale-dependent effective average action is O(N) invariant for both the transformations of the background and the fluctuation field. Due to the cutoff action, however, the EAA becomes a genuine bi-field functional, which motivated the introduction of a separat scaling parameter for the fluctuation fields.
The beta functions were derived in two steps by matching operators on both sides of the flow equation (or its second derivative) evaluated at the base point. For this purpose the flow equation was expanded in powers of a derivative operator and off-diagonal elements of a heat kernel expansion were applied. The consistency of the formalism was underlined by the appearance of nontrivial relations between the renormalization flow of background and fluctuation operators.
In the restricted subspace of couplings, where L_2 is set to zero, a fixed point for all N emerges. It exhibits one relevant direction, which is already present in an one-parameter truncation. The inclusion of further couplings (L_1 and α) only adds irrelevant directions, but it is required to become sensitive to the N-dependence of

the critical exponents. The results for ν in the truncation $\{\zeta, \alpha, L_1\}$ agree qualitatively with the pre-existing literature, but show some numerical difference that is likely due to the limited truncation ansatz. The presence of a nontrivial fixed point was verified in various approximations and choices of the coarse-graining scheme. However, this fixed point is lost in a truncation which includes the coupling L_2. This can be due to the limited truncation considered and the quadratic structure of the computed beta functions, or it is maybe related to more subtle conceptual issues, of which one will be discussed in Sec. 4.1.

The results of the FRG calculations were finally compared to lattice computations as an alternative non-perturbative tool to study field theories. The Monte Carlo RG was depicted which bases on the idea of block spin transformations. Starting with specific coupling values on a large lattice, configurations are generated on which optimized block spin transformations are performed subsequently. From these blocked configurations corresponding effective couplings can be determined by the demon method and can be related to the initial couplings in order to obtain the renormalization flow of the theory. In comparison to the FRG computations, explicit simulations were performed for an ansatz up to fourth order in the derivatives. The results of these simulations are preliminary, but they already show qualitive agreement between MCRG and FRG. The quantitative deviations can be explained by differences in the truncation procedure. The MCRG finds a stable fixed point even if one includes all fourth-order operators and it hence strongly supports the assumpation that the nonlinear $\mathrm{O}(N)$ models are non-perturbatively renormalizable. The outlined procedure provides the means to study the renormalization flow of theories by numerical simulations and can serve in this way as a useful complementation of FRG calculations.

4. Renormalization of the Hamiltonian Action

The analysis presented in this chapter was developed in collaboration with Gian Paolo Vacca and Luca Zambelli.

4.1. Modification of the Path Integral Measure

The aim of this chapter is to analyze nonlinear sigma models from a "Hamiltonian point of view", which means that the investigations will be based on a descripition of the theory in terms of phase space coordinates. Before a functional RG formalism will be developed for a Hamiltonian action functional in Sec. 4.2, the interplay between the path integral measure and the regularization procedure of standard FRG shall be discussed first. This relation was pointed out in [22] and the main argument will be briefly depicted here for the simple example of quantum mechanics, before possible consequences for the calculations of nonlinear field theories like in Chap. 3 are discussed.

The path integral formulation is usually derived by starting from canonical quantization and integrating out the momenta at some point. This integration is, however, not a necessary step and it is interesting to study to what the introduction of the FRG regulator corresponds to on this level:

$$Z_k[J] = \int \mathcal{D}q \ \mu[q] \ \mathrm{e}^{-\int_t \partial_t q \, \partial_t q + V(q) + \frac{1}{2} q R_k q - Jq} \tag{4.1}$$

$$= \int \mathcal{D}q\mathcal{D}p \ \mu[q,p] \ \mathrm{e}^{\ \int_t \mathrm{i}\, p \left(1+\frac{R_k}{-\partial_t^2}\right)^{1/2} \partial_t q - \frac{1}{2}p^2 - V(q) \ + Jq} \ . \tag{4.2}$$

Note that t denotes the time coordinate in this section (only). The cutoff action of FRG apparently corresponds to a modification of the Legendre term $p(t)\partial_t q(t)dt$. But this term and the path integral measure are directly related to the structure of the phase space. The Legendre term is the pullback of the Liouville one-form $\lambda = pdq$ and the measure $d\lambda = dpdq$ is the exterior derivative. A modification depending on

k should hence affect both objects in a balanced way. The appropriate modification of the path integral measure is given by

$$\mu \to \mu_k = \mu \cdot \det{}^{1/2} \left(1 + \frac{R_k}{-\partial_t^2} \right) \tag{4.3}$$

This k-dependence of the measure can also be understood from another point of view. It was mentioned in Sec. 2.4 that the cutoff action has the structure of a Gaußian integral which becomes a rising δ-function for $k \to \infty$ due to the divergence of R_k. This representation of the δ-distibution as a limit of a Gaußian integral, however, requires an appropriate normalization which is proportional to $\det^{1/2} R_k$ for $k \to \infty$. The measure (4.3) provides this regularization, while it yields at the same time the correct limit $\mu_{k\to 0} = \mu$ (up to an irrelevant factor).
The important aspect of this modification of the measure is that it alters the flow equation of FRG. Absorbing the k-dependent factor in (4.3) into the action functional and taking the derivative $k\partial_k$, it is straightforward to derive that the flow equation (2.33) reveices an additional term:

$$k\partial_k \Gamma_k = \frac{1}{2} \mathrm{Tr} \left\{ \frac{k\partial_k R_k}{\Gamma^{(2)} + R_k} \right\} - \frac{1}{2} \mathrm{Tr} \left\{ \frac{k\partial_k R_k}{-\partial_t^2 + R_k} \right\} . \tag{4.4}$$

As long as the regulator R_k is field-independent, this term only contributes to the renormalization of the vacuum energy. The computations of Sec. 3.2-3.4, however, are based on a background field expansion and a regulator which depends on the base-point. It is hence worthwhile to investigate if and how these calculations are affected by a modification of the measure. This is in fact a very difficult task, since the action functional in configuration space contains infinitely many nontrivial terms, see (3.10) and (3.11), such that a direct argumentation via a corresponding Hamiltonian formulation of the expanded functional is impossible. Instead, one has to use the normalization of the rising δ-function as guideline, which leads to the ansatz

$$\mu_k = \mu \cdot \det{}^{1/2} \left(1 + \frac{R_k}{\zeta \Delta} \right) , \quad \text{with } \Delta = -\nabla_\mu \nabla^\mu . \tag{4.5}$$

The covariant Laplacian serves as natural scale for the regulator. This choice can also be understood, if one follows the reasoning [96] that the measure of the path integral ought to be proportional to $\det^{1/2} S^{(2)}$, where S is the bare action. The Hessian of the full expanded action is too complicated, but one could regard the kinetic operator of the fluctuations as a rough, first approximation which ignores the further interaction terms[1]. In this sense the denominator in (4.5) is chosen such that it cancels with $\det^{1/2}(\zeta\Delta)$ in μ and hence provides the correct normalization $\mu_{k\to\infty} = \det^{1/2} R_k$. Since the couplings in μ are bare ones, the ζ in the denominator should be understood as bare coupling ζ_Λ as well. Using the ansatz (4.5), the additional term in the flow equation (3.14) can be computed in the way mentioned above and reads

$$-\frac{1}{2}\,\mathrm{Tr}\left\{\frac{k\partial_k R_k}{\zeta_\Lambda\Delta + R_k}\right\}. \tag{4.6}$$

One can deal with this trace by the same means that has been used in Sec. 3.3. The result is proportional to the first trace in (3.29), but multiplied with a slightly modified $Q_{\frac{d}{2}-2,1}$- functional (3.31) which depends on a function $\hat{f}(z)$ which is similar to (3.25), but has the denominator $R_k(z) + \zeta_\Lambda z$ instead of P_k.

If one includes this term in the computation of Sec. 3.2-3.4, it leads to interesting results: Note that the heat kernel expansion of (4.6) yields according to (3.29) no second-order terms, but only operators of fourth order in the derivatives which affect the running of L_1 and L_2. As a consequence of this contribution, the full fourth-order truncation, including the problematic coupling L_2, in fact stabilizes and a nontrivial fixed point can be identified for each N. Similar to the results in the reduced truncations, the critical ζ^* increases with N and the critical couplings L_1^* and L_2^* are small in comparison to ζ^*, with $L_1^* < 0$ and $L_2^* > 0$. Furthermore, this fixed point has only one IR-relevant direction in accordance with previous investigations of the model and the MCRG computations. However, the critical exponent Θ^R corresponding to the relevant direction deviates strongly from the literature values for $\nu(N) = 1/\Theta^R$. While Θ^R is supposed to be roughly of the form $1 + \frac{1}{N}$, these computations yield a critical exponent which is approximately four times too large and converges to 4.228 for $N \to \infty$ instead of 1.

Note that a k-dependent coupling ζ_k in the denominator of (4.5) was explicitly checked as an alternative modification of the measure, arguing that it still provides the appropriate asymptotics due to $\zeta_k \to \zeta_\Lambda$ for $k \to \infty$. However, this alternative does not improve the computations, but, on the contrary, becomes unstable again if one includes L_2.

In order to clearify if a modification of the measure is really the necessary ingredient to stabilize the covariant FRG computations of the nonlinear O(N) model, a refined analysis is required how the path integral measure ought to be defined correctly in nonlinear theories which are formulated in terms of a background field expansion.

[1] One could argue that the kinetic term of the fluctuations also includes $\alpha\Delta^2$, but since this discussion focuses on the nontrivial fixed point with $\alpha^* = 0$, this operator can be neglected. It was explicitly checked, yet, that an inclusion would not change the result $\alpha^* = 0$.

This, however, constitutes a very difficult task, which will not be addressed here. Instead, the "Hamiltonian point of view" shall be explored further by a Hamiltonian formulation of the FRG.

4.2. Renormalization of the Average Effective Hamiltonian Action

In most explicit computations the Lagrangian formulation of quantum field theory is favored against the Hamiltonian one, since the latter has to deal with an increased number of variables while loosing Lorentz covariance. For some questions, however, the Hamiltonian formulation is more suitable or can provide additional insights. A recent example is the use of Hamiltonian approaches in non-Abelian gauge theories, cf. for instance[2] [109] or [110],[111],[108].

Most recently, Gian Paolo Vacca and Luca Zambelli developed an alternative approach to QFT which is formulated in terms of phase space variables and describes the renormalization of the effective Hamiltonian action following the ideas of the FRG. While a detailed presentation is given in [23], a brief overview of the formalism for the case of a scalar field theory shall be provided here, before the application to sigma models is presented in the next section. The main motivation[3] for the investigation of the effective Hamiltonian action is the possibility to study alternative ansätze for the effective action functional, e.g. non-quadratic functionals of the canonical momenta. It hence provides alternative expansion schemes for the truncation of the effective average action. This will be demonstrated in the subsequent section.

Note that the discussion in this chapter is developed in Minkowski spacetime[4], since it is the more natural setting for the Hamiltonian formalism. Note furthermore that a "mostly plus" signature is used.

In order to describe the Average Effective Hamiltonian Action formalism, the functional relations of the effective Hamiltonian action shall be explained first, before a regularization is introduced and a flow equation is derived. The description is

[2] The Hamiltonian flow derived in [108] should not be confused with the flow equation in this chapter which is formulated in phase space while [108] is based on a wave functional representation of quantum states.

[3] Moreover, the path integral measure simplifies in phase space. However, if one introduces the Lorentz-covariant Hamiltonian as it is done here, this advantage gets lost again. One could consider a reduction of the phase space to longitudinal modes, but so far no projection has been found that is covariant w.r.t. diffeomorphisms of the target manifold, see the remark in Sec. 4.3.

[4] although a formulation in Euclidean space is possible as well

given for scalar fields, which can be for example the coordinates in the nonlinear spaces that were already discussed. The related target space indices, however, will be suppressed in this section for the sake of brevity. A definion of the action and the partition sum in terms of phase space variables is simply given by

$$S[\varpi,\varphi] = \int d^d x \; \varpi\, \partial_t \varphi - \mathcal{H}\big(\varpi,\varphi\big) \tag{4.7}$$

$$Z[I,J] = \mathrm{e}^{\mathrm{i}\, W[I,J]} = \int \mathcal{D}\varpi \mathcal{D}\varphi \, \mu[\varpi,\varphi]\, \mathrm{e}^{\mathrm{i}\left(S[\varpi,\varphi]+I\cdot\varpi+J\cdot\varphi\right)}\,, \tag{4.8}$$

where ϖ denotes the canonical momenta, $\mathcal{H}$ the Hamiltonian density and $\cdot$ represents as in Sec. 2.4 the inner product of the Hilbert space. Analogous to the Lagrangian formalism, the effective Hamiltonian action $\Gamma[\pi,\phi]$ is defined as Legendre transform

$$\Gamma[\pi,\phi] = \operatorname*{ext}_{I,J} \big\{ W[I,J] - I\cdot\pi - J\cdot\phi \big\}\,. \tag{4.9}$$

It immediately follows that π and ϕ are the expectation values of the quantum fields:

$$\pi = \frac{\delta W}{\delta I} = \big\langle \varpi \big\rangle\,, \quad \phi = \frac{\delta W}{\delta J} = \big\langle \varphi \big\rangle\,. \tag{4.10}$$

With the relations

$$I = -\frac{\delta\Gamma[\pi,\phi]}{\delta\pi}\,, \quad J = -\frac{\delta\Gamma[\pi,\phi]}{\delta\phi}\,, \tag{4.11}$$

for the source terms one can express the effective Hamiltonian action by the integro-differential equation:

$$\mathrm{e}^{\mathrm{i}\Gamma[\pi,\phi]} = \int \mathcal{D}\varpi \mathcal{D}\varphi \, \mu[\varpi,\varphi]\, \mathrm{e}^{\mathrm{i}\left(S[\pi,\varphi] - \frac{\delta\Gamma}{\delta\phi}\cdot(\varphi-\phi) - \frac{\delta\Gamma}{\delta\pi}\cdot(\varpi-\pi)\right)}\,. \tag{4.12}$$

It is important to stress that the effective Hamiltonian action provides a complete description of a quantum theory and contains the entire information of the effective (Lagrangian) action, which is related to the former by

$$\Gamma[\phi] = \operatorname*{ext}_{\pi} \Gamma[\pi,\phi]\,. \tag{4.13}$$

It is straightforward (in case of a Hamiltonian which is quadratic in the momenta) to verify that (4.13) yields the correct expression for the Lagrangian effective action: The source I vanishes according to (4.11) and the Gaußian integral of the momenta leads to the standard Lagrangian.

The standard Hamiltonian formalism assigns a special rôle to the time direction and is hence not Lorentz-covariant. It is possible to perform Lorentz-invariant computations, but these usually require explicits checks which quickly become inconvenient. It is therefore reasonable to use a manifestly invariant framework right from the start and extend the Hamiltonian formalism outlined above to a covariant one. In case of a Hamiltonian which is quadratic in the momenta, this simply amounts to the introduction of $d-1$ Gaußian integrals in the path integral (4.8). Note that in nonlinear theories a nontrivial path integral measure comes along with these Gaußian integrals. This effect will be taken into account in the derivation of the flow equation, but it will be irrelevant in the explicit calculations in the following section and can be neglected there. All relations (4.7) to (4.13) remain true for such a covariant extension if one applies the simple replacement

$$\pi \to \pi^{\nu}, \quad I \to I^{\nu} . \tag{4.14}$$

In order to regularize the quantum theory and analyze its renormalization, one can follow the reasoning outlined in Sec. 2.4. The regularization is implemented by the introduction of a cutoff action

$$Z_k[I^{\nu}, J] = \mathrm{e}^{\mathrm{i}\, W_k[I^{\nu},J]} = \int \mathcal{D}\varpi_{\nu}\mathcal{D}\varphi\, \mu_k\, \mathrm{e}^{\mathrm{i}\left(S[\varpi_{\nu},\varphi]+\Delta S_k[\varpi_{\nu},\varphi]+I^{\nu}\cdot\varpi_{\nu}+J\cdot\varphi\right)} \tag{4.15}$$

$$\Delta S_k[\varpi_{\nu}, \phi] = -\int d^d x\ \varpi_{\nu}\, R_k^{\pi}(-\partial^2)\, \partial^{\nu}\varphi\,. \tag{4.16}$$

The quadratic form of the cutoff action will ensure a comparably simple structure of the resulting flow equation, while it simultanously regulates ϖ as well as φ for an appropriate choice of R_k^{π}. The mass dimension of this regulator is smaller than the one of the standard FRG regulator, but it has to fulfill the same constraints (2.30). Owing to these properties the cutoff action suppresses the modes below the scale k and leads to a gradual integration of momentum shells as R_k^{π} decreases while k is lowered. Note that only field-independent regulators will be considered in this thesis.

Based on the regularized path integral (4.15) one can define the *Average Effective Hamiltonian Action* (AEHA) $\Gamma_k\,[\pi_{\nu}, \phi]$ as the modified Legendre transform

$$\Gamma_k\,[\pi_{\nu}, \phi] + \Delta S_k\,[\pi_{\nu}, \phi] = \operatorname*{ext}_{J,I^{\nu}} \left\{ W_k[I^{\nu}, J] - I^{\nu}\cdot\pi_{\nu} - J\cdot\phi \right\}. \tag{4.17}$$

One can immediately derive expressions for the sources

$$J = -\frac{\delta\Gamma_k}{\delta\phi} - R_k^{\pi}\,\partial^{\nu}\pi_{\nu}\,, \quad I^{\nu} = -\frac{\delta\Gamma_k}{\delta\pi_{\nu}} + R_k^{\pi}\,\partial^{\nu}\phi \tag{4.18}$$

and use these to obtain an integro-differential equation for the AEHA:

$$\mathrm{e}^{\mathrm{i}\Gamma_k[\pi_\nu,\phi]} = \int \mathcal{D}\varpi_\nu \mathcal{D}\varphi\, \mu_k\, \mathrm{e}^{\mathrm{i}\left(S[\varpi_\nu,\varphi]+\Delta S_k[(\varpi-\pi)_\nu,\varphi-\phi]-\frac{\delta\Gamma_k}{\delta\pi_\nu}\cdot(\varpi-\pi)_\nu-\frac{\delta\Gamma_k}{\delta\phi}\cdot(\varphi-\phi)\right)}\,. \tag{4.19}$$

Owing to the properties of the regulator, the AEHA interpolates between the bare action in the UV[5] and the full effective action in the IR:

$$\Gamma[\pi_\nu,\phi] \xleftarrow{k\to 0} \Gamma_k[\pi_\nu,\phi] \xrightarrow{k\to\infty} S[\pi_\nu,\phi]\,. \tag{4.20}$$

The $k \to 0$ limit is trivial, since the regulator simply vanishes. In the $k \to \infty$ limit, the cutoff action (accompanied by an appropriate regulator-dependent normalization in the measure) serves as a rising δ-function for each component $(\varphi-\phi)^a$ and $p_\nu(\varpi-\pi)_a^\nu$ in target space, where p denotes the Fourier variable if one performs such transform. The emergence of these constraints is explicitly demonstrated for a simple example in [23] and can be understood very intuitively, since the diverging regulator suppresses all modes apart from the ones for which $(\varphi-\phi)^a$ and $p_\nu(\varpi-\pi)_a^\nu$ are identically zero. The rising constraint for the momenta applies only to the longitudinal modes, as the cutoff action completely vanishes for all transverse modes with $p^\nu \perp (\varpi-\pi)_a^\nu$. However, it is straightforward to check by a successive integration of the quantum momenta ϖ that in case of a bare Hamiltonian which is quadratic in the momenta the coincidence limit $\varpi^\mu \to \pi^\mu$ is effectively given also for the transverse modes in the path integral. With $\varpi^\mu \to \pi^\mu$ and $\varphi \to \phi$, the appropriate limit $\Gamma_k[\pi_\nu,\phi] \xrightarrow{k\to\infty} S[\pi_\nu,\phi]$ is ensured.

In order to investigate the effective action, a flow equation for the AEHA can be derived in a similar way as for the EAA. The derivative of (4.19) w.r.t. the logarithm of the momentum scale yields

$$\mathrm{i}\dot{\Gamma}_k[\pi_\nu,\phi] = \frac{\dot{\mu}_k}{\mu_k} - \mathrm{i}\int d^dx\, \left\langle(\varpi-\pi)_\nu \dot{R}_k^\pi\, \partial^\nu(\varphi-\phi)\right\rangle_k\,. \tag{4.21}$$

The r.h.s. of this equation can be expressed in terms of R_k^π and Γ_k, if one employs the relations (4.18) for the source terms and rewrites the connected two-point functions

[5]Note that it, once again, implicitly assumed that a fundamental theory exist such that the limit $\Lambda \to \infty$ can be performed.

as follows (by suppressing the indices for the sake of convenience)

$$
\begin{aligned}
&\mathrm{i}\Big\langle \mathcal{T}\begin{pmatrix} (\varpi-\pi)\otimes(\varpi-\pi) & (\varpi-\pi)(\varphi-\phi) \\ (\varphi-\phi)(\varpi-\pi) & (\varphi-\phi)(\varphi-\phi)\end{pmatrix}\Big\rangle_k = W_k^{(2)}[I,J] = \begin{pmatrix} \frac{\delta W_k}{\delta I}\otimes\frac{\overleftarrow{\delta}}{\delta I} & \frac{\delta^2 W_k}{\delta J\delta I} \\ \frac{\delta^2 W_k}{\delta I\delta J} & \frac{\delta^2 W_k}{\delta J\delta J}\end{pmatrix} \\
&= \begin{pmatrix} \pi\otimes\frac{\overleftarrow{\delta}}{\delta I} & \frac{\delta\pi}{\delta J} \\ \frac{\delta\phi}{\delta I} & \frac{\delta\phi}{\delta J}\end{pmatrix} = \begin{pmatrix} I\otimes\frac{\overleftarrow{\delta}}{\delta\pi} & \frac{\delta I}{\delta\phi} \\ \frac{\delta J}{\delta\pi} & \frac{\delta J}{\delta\phi}\end{pmatrix}^{-1} = -\begin{pmatrix} \frac{\delta\Gamma_k}{\delta\pi}\otimes\frac{\overleftarrow{\delta}}{\delta\pi} & \frac{\delta^2\Gamma_k}{\delta\phi\delta\pi} - R_k^\pi\partial \\ \frac{\delta^2\Gamma_k}{\delta\pi\delta\phi} + R_k^\pi\partial & \frac{\delta^2\Gamma_k}{\delta\phi\delta\phi}\end{pmatrix}^{-1} \qquad (4.22) \\
&\equiv -\begin{pmatrix} A & B \\ \tilde{B} & D\end{pmatrix}^{-1} = -\begin{pmatrix} A^{-1}+A^{-1}B(D-\tilde{B}A^{-1}B)^{-1}\tilde{B}A^{-1} & -A^{-1}B(D-\tilde{B}A^{-1}B)^{-1} \\ -(D-\tilde{B}A^{-1}B)^{-1}\tilde{B}A^{-1} & (D-\tilde{B}A^{-1}B)^{-1}\end{pmatrix}
\end{aligned}
$$

This directly leads to the flow equation of the Average Effective Hamiltonian Action:

$$
\begin{aligned}
\mathrm{i}\dot{\Gamma}_k[\pi,\phi] = \frac{\dot{\mu}_k}{\mu_k} - \mathrm{Tr}\Bigg\{ &\left(\frac{\delta^2\Gamma_k}{\delta\pi\delta\phi} + R_k^\pi\partial\right)^{\nu}\left(\frac{\delta^2\Gamma_k}{\delta\pi\delta\pi}\right)^{-1}_{\nu\mu}\dot{R}_k^\pi\partial^\mu \qquad (4.23) \\
&\left[\frac{\delta^2\Gamma_k}{\delta\phi\delta\phi} - \left(\frac{\delta^2\Gamma_k}{\delta\pi\delta\phi} + R_k^\pi\partial\right)^{\mu}\left(\frac{\delta^2\Gamma_k}{\delta\pi\delta\pi}\right)^{-1}_{\mu\nu}\left(\frac{\delta^2\Gamma_k}{\delta\phi\delta\pi} - R_k^\pi\partial\right)^{\nu}\right]^{-1}\Bigg\}
\end{aligned}
$$

Since only field-independent regulators are considered in this chapters, the additional term in the flow equation only describe the renormalization of the vacuum energy and will hence be neglected in the following.

4.3. Applications to Sigma Models

In order to further investigate the new Hamiltonian formulation of the FRG, one should study its application to test models. Before the interesting case of a nonlinear sigma model will be examined in more detail, a brief consistency check is provided by a simple computation of the linear sigma model. Suppressing spacetime and target space indices again for the sake of brevity, the simple truncation[6]

$$
\Gamma_k[\pi,\phi] = \int d^dx\ \tfrac{1}{2}\,\pi^\mu\pi_\mu - \pi^\mu\partial_\mu\phi - V_k(\phi)\,, \qquad (4.24)
$$

[6] Remember that a "mostly plus" signature of Minkowski spacetime is used in this chapter.

is considered, which corresponds to the local potential approximation in standard FRG. The second derivatives of the action functional then read

$$\frac{\delta^2\Gamma_k}{\delta\phi\delta\phi} = -\frac{\delta^2 V_k}{\delta\phi\delta\phi}\,, \quad \frac{\delta^2\Gamma_k}{\delta\pi_\mu\delta\phi} = \partial^\mu\,, \quad \frac{\delta^2\Gamma_k}{\delta\pi_\mu\delta\pi_\nu} = \eta^{\mu\nu}\,. \tag{4.25}$$

The flow equation (4.23) simplifies to

$$\mathrm{i}\dot{\Gamma}_k[\pi,\phi] = -\frac{1}{2}\mathrm{Tr}\left\{(R_k^\pi\partial+\partial)^\nu\,\dot{R}_k^\pi\partial_\nu\left[-\frac{\delta^2 V_k}{\delta\phi\delta\phi} + (R_k^\pi\partial+\partial)^\mu\,(R_k^\pi\partial+\partial)_\mu\right]^{-1}\right\}. \tag{4.26}$$

It is convenient to apply a Fourier transform and to introduce the operator $\Omega_k^\mu(p)$:

$$\Omega_k^\mu(p) = R_k^\pi(p^2)\,p^\mu + p^\mu \tag{4.27}$$

$$\Rightarrow\quad \mathrm{i}\dot{\Gamma}_k[\pi,\phi] = -\mathrm{Tr}\left\{\Omega_k^\mu\,\dot{\Omega}_{k,\mu}\left[\frac{\delta^2 V_k}{\delta\phi\delta\phi} + \Omega_k^\mu\,\Omega_{k,\mu}\right]^{-1}\right\}. \tag{4.28}$$

If one chooses

$$\Omega_k^\mu(p) = p^\mu + \left(k\frac{p^\mu}{p} - p^\mu\right)\Theta(k^2-p^2)\,, \tag{4.29}$$

with $p = \sqrt{p^\mu p_\mu}$, the flow equation becomes

$$\mathrm{i}\dot{\Gamma}_k[\pi,\phi] = -\frac{1}{2}\mathrm{Tr}\left\{\dot{R}_k\left[\frac{\delta^2 V_k}{\delta\phi\delta\phi} + p^2 + R_k\right]^{-1}\right\}, \tag{4.30}$$

where R_k denotes the optimized regulator (2.34) which is related to Ω_k by $R_k = \Omega_k^2 - p^2$ and $\dot{R}_k = 2\Omega_k^\mu\dot{\Omega}_{k,\mu}$. Performing the analytic continuation $p_0 \to \mathrm{i}p_4$ of (4.30), one obtains the same flow equation for the potential V_k as given by the standard FRG formalism in Euclidean spacetime (if one takes into account the sign convention in (4.24)). The choice (4.29) or $R_k^\pi = \left(\frac{k}{p}-1\right)\Theta(k^2-p^2)$ can obviously be understood as the Hamiltonian version of the optimized regulator and will be used also in the following calculations.

While the Hamiltonian formalism simply agrees with the Lagrangian one for simple linear models, it really becomes interesting in nonlinear theories. An operator of the kind $h^{ab}(\phi)\,\pi_a^\mu\pi_{b,\mu}$ constitutes a nontrivial interaction of the fields π and ϕ and naturally generates operators of higher order in π. The test case for the application of the AEHA scheme to such theories will be the nonlinear O(N) models, which have already been discussed in much detail by the alternative non-perturbative methods of MCRG and standard Lagrangian FRG and whose critical properties provide a useful benchmark.

Even though a covariant calculation of the renormalization flow would be desirable, the extension of background field methods as they were used in Sec. 3.2 to phase space coordinates is nontrivial and would require a lot of additional consideration. The calculations in thesis will therefore be performed in a specific parametrization which is convenient from a computational point of view. For our purposes the stereographic coordinates are particular efficient. The metric is given as

$$h_{ab}(\phi) = (1+\boldsymbol{\phi}^2)^{-2}\delta_{ab}\,, \quad h^{ab}(\phi) = (1+\boldsymbol{\phi}^2)^{2}\delta_{ab}\,, \quad \text{with } \boldsymbol{\phi}^2 = \sum_{a=1}^{N-1} \phi^a\phi^a\,. \tag{4.31}$$

Note that for remainder of this chapter the square $\boldsymbol{v}^2$ of any $(N-1)$-tuple v^a or v_a with (upper or lower) target space indices will denote this kind of sum. Working in this coordinate frame, the ansatz

$$\Gamma_k[\pi,\phi] = \int d^dx\; V_k(Z) - \pi_a^\mu \partial_\mu \phi^a \tag{4.32}$$

shall be studied in more detail, where $V_k(Z)$ is a generic function of

$$Z \equiv \tfrac{1}{2}\, h^{ab}(\phi)\, \pi_a^\mu \pi_{b,\mu}\,. \tag{4.33}$$

Owing to the Legendre term $\pi_a^\mu\partial_\mu\phi^a$, the usual kinetic term $h_{ab}\partial_\mu\phi^a\partial^\mu\phi^b$ of the Lagrangian formalism will be generated in the effective Hamiltonian action as well, and one could consider the inclusion of this operator in the ansatz. Furthermore, the Legendre term itself could be renormalized. However, a tedious but straightforward computation of this generalization of (4.32) explicitly showed that a potentiell scaling parameter of the Legendre term would not run at all, and the renormalization of the standard kinetic term is directly proportional to the renormalization of the coupling g_k in the simple ansatz $V(Z) = g_k\, Z$. This is no surprise, since both operators are related to each other by the Legendre transform of the bare action. The following analysis will thus just focus on the running of $V_k(Z)$, which will be called "momentum potential".

In order to project the flow equation (4.23) on $\dot{V}_k$, it can be evaluated at constant ϕ. In fact, the most convenient choice is a vanishing field configuration $\phi \to 0$. The structure of the computation simplifies considerably while no information about $\dot{V}_k(Z)$ is lost, since this is a function of Z only which does not vanish for $\phi \to 0$, but is equal to $\frac{1}{2}\boldsymbol{\pi}_\mu^2 \left(\equiv \frac{1}{2}\boldsymbol{\pi}^2\right)$. Note that all terms which are generated in the flow equation can be uniquely decomposed into three different types of operators: 1. Covariant expressions in terms of the operator Z, 2. other covariant expressions which include operators that are not considered in the chosen truncation (like e.g. $h^{ab}\pi_a^\mu\pi_b^\nu\ h^{cd}\pi_{c,\mu}\pi_{d,\nu}$), or 3. terms which break the reparametrization invariance, but vanish for $\phi \to 0$. A simple example is $(1+\phi^2)\delta^{ab}\pi_a^\mu\pi_{b,\mu} = Z - \phi^2(\phi^2+1)\delta^{ab}\pi_a^\mu\pi_{b,\mu}$. The evaluation at $\phi \to 0$ thus provides the required projection on covariant operators, which constitute the actual physical content of the theory. The generation of terms which break reparametrization invariance is just an artefact of the calculations.

The second functional derivatives evaluated at $\phi = 0$ read[7]

$$\left.\frac{\delta^2\Gamma_k}{\delta\pi_b^\nu\delta\pi_a^\mu}\right|_{\phi=0} = V_k'(Z)\,\delta^{ab}\eta_{\mu\nu} + \pi_{a,\mu}\pi_{b,\nu}\,V_k''(Z)\,, \tag{4.34}$$

$$\left.\frac{\delta^2\Gamma_k}{\delta\phi^b\delta\pi_a^\mu}\right|_{\phi=0} = -\partial_\mu\delta^a{}_b\,, \qquad \left.\frac{\delta^2\Gamma_k}{\delta\pi_b^\mu\delta\phi^a}\right|_{C_0} = \partial_\mu\delta^b{}_a\,, \tag{4.35}$$

$$\left.\frac{\delta^2\Gamma_k}{\delta\phi^b\delta\phi^a}\right|_{\phi=0} = 4\,Z\,V_k'(Z)\,\delta_{ab}\,. \tag{4.36}$$

By means of the projectors

$$\Pi_{\parallel}{}^{ab}_{\mu\nu}(\pi) = \frac{\pi_a^\mu\pi_b^\nu}{\boldsymbol{\pi}^2} = \frac{\pi_a^\mu\pi_b^\nu}{2Z}\,, \quad \Pi_{\perp}{}^{\mu\nu}_{ab} = \delta_{ab}\eta^{\mu\nu} - \frac{\pi_a^\mu\pi_b^\nu}{\boldsymbol{\pi}^2}\,, \tag{4.37}$$

the inverse of $\delta^2_{\pi\pi}\Gamma_k$ can be written as

$$\left(\left.\frac{\delta^2\Gamma_k}{\delta\pi^2}\right|_{\phi=0}\right)^{-1} = V_k'^{-1}\,\Pi_\perp(\pi) + (V_k' + 2ZV_k'')^{-1}\,\Pi_\parallel(\pi)\,. \tag{4.38}$$

If ones applies a Fourier transform and utilizes the notation (4.27), the flow equation (4.23) for the momentum potential (4.32) becomes

$$\mathrm{i}\dot{V}_k(Z) = \mathrm{Tr}\left\{\frac{\Omega_k^\mu(p)\left[V_k'^{-1}\Pi_\perp(\pi) + (V_k'+2ZV_k'')^{-1}\Pi_\parallel(\pi)\right]_{\mu\nu}\dot{\Omega}_k^\nu(p)}{4ZV_k' - \Omega_k^\mu(p)\left[V_k'^{-1}\Pi_\perp(\pi) + (V_k'+2ZV_k'')^{-1}\Pi_\parallel(\pi)\right]_{\mu\nu}\Omega_k^\nu(p)}\right\} \tag{4.39}$$

$$= \mathrm{Tr}\left\{\frac{V_k'^{-1}\,\Omega_k^\mu\dot{\Omega}_{k,\mu}\,\delta_{ab} - \frac{V_k''}{V_k'(V_k'+2ZV_k'')}(\Omega\pi)_a(\dot{\Omega}\pi)_b}{\left(4ZV_k' - V_k'^{-1}\Omega_k^\mu\Omega_{k,\mu}\right)\delta_{ba} + \frac{V_k''}{V_k'(V_k'+2ZV_k'')}(\Omega\pi)_b(\Omega\pi)_a}\right\}\,. \tag{4.40}$$

Using projectors in the same way as above with $(\Omega\pi)_a = (\Omega^\mu\pi_\mu)_a$ instead of π_a^μ, one can find an expression like (4.38) in target space for the denominator of (4.40).

[7] The spacetime indices are again suppressed.

Taking the trace in target space finally yields

$$\mathrm{i}\dot{V}_k(Z) = \int_p \frac{(N-2)\Omega_k^\mu \dot{\Omega}_{k,\mu}}{4ZV_k'^2 - \Omega_k^\mu \Omega_{k,\mu}} + \frac{\Omega_k^\mu \dot{\Omega}_{k,\mu} - \frac{V_k''}{V_k'+2ZV_k''}(\Omega\pi)_a(\dot{\Omega}\pi)_b\delta^{ab}}{4ZV_k'^2 - \Omega_k^\mu \Omega_{k,\mu} + \frac{V_k''}{V_k'+2ZV_k''}(\Omega\pi)^2}\,. \tag{4.41}$$

Having an exact equation for the renormalization of a generic momentum potential, one can now study it for specific ansätze. The simplest ansatz is

$$V_k(Z) = g_k\, Z\,, \tag{4.42}$$

and should be checked first. The flow equation strongly simplifies in this case:

$$\mathrm{i}\dot{V}_k(Z) = \int_p \frac{(N-1)\,\Omega_k^\mu \dot{\Omega}_{k,\mu}}{4Zg_k^2 - \Omega_k^\mu \Omega_{k,\mu}} \quad \overset{\frac{d}{dZ}()|_{Z=0}}{\Longrightarrow} \quad \dot{g}_{1,k} = \mathrm{i}\int_p \frac{4\,g_k^2\,(N-1)\,\Omega_k^\mu \dot{\Omega}_{k,\mu}}{(\Omega_k^\mu \Omega_{k,\mu})^2} \tag{4.43}$$

If one chooses the optimized regulator (4.29), the evaluation of the integral by means of analytic continuation $p_0 \to \mathrm{i}p_4$ yields the beta function

$$\beta_g = -\frac{4\,k^{d-2}(N-1)}{(4\pi)^{d/2}\,\Gamma(d/2+1)} g_k^2\,. \tag{4.44}$$

Note that g_k corresponds in case of the simple ansatz (4.42) directly to the equally denoted $g_k = \zeta_k^{-1}$ in the simplest Lagrangian truncation of the nonlinear sigma model, that was discussed in [43]. In fact, (4.44) agrees with the result therein (up to a scheme-dependent numerical factor) and hence provides a further consistency check of the AEHA. The result contains a nontrivial fixed point for $d > 3$, but the critical properties of the model in three dimensions are not correctly reproduced as discussed in Chap. 3. The covariant calculation within the Lagrangian FRG requires for this purpose a truncation which includes operators of fourth order in the derivatives. In order to compare both formulations it is interesting to study in which way an enlargement of the Hamiltonian ansatz improves the computations.
If one uses the optimized regulator (4.29) for the analysis, the running (4.41) of a generic momentum potential simplifies to

$$\begin{aligned}\mathrm{i}\dot{V}_k(Z) &= \int_p \Theta(k^2-p^2)\left(\frac{(N-2)k^2}{4ZV_k'^2 - k^2} + \frac{k^2 - \frac{V_k''}{V_k'+2ZV_k''}\frac{k^2}{p^2}p_\mu p_\nu\,\pi_a^\mu \pi_b^\nu \delta^{ab}}{4ZV_k'^2 - k^2 + \frac{V_k''}{V_k'+2ZV_k''}\frac{k^2}{p^2}p_\mu p_\nu\,\pi_a^\mu \pi_b^\nu \delta^{ab}}\right)\\ &= \int_p \Theta(k^2-p^2)\left(\frac{(N-2)k^2}{4ZV_k'^2 - k^2} - 1 + \frac{4ZV_k'^2}{4ZV_k'^2 - k^2 + \frac{V_k''}{V_k'+2ZV_k''}\frac{k^2}{p^2}p_\mu p_\nu\,\pi_a^\mu \pi_b^\nu \delta^{ab}}\right)\end{aligned} \tag{4.45}$$

The Fourier integral can be performed if one expands the last term in $\pi_\mu \pi_\nu$

$$\mathrm{i}\dot{V}_k(Z) = \int_p \Theta(k^2 - p^2) \left(\frac{(N-1)k^2}{4ZV_k'^2 - k^2} \right. \tag{4.46}$$
$$\left. + \sum_{n=1}^{\infty} \frac{(-1)^n \, 4ZV_k'^2}{(4ZV_k'^2 - k^2)^{n+1}} \left(\frac{V_k''}{V_k' + 2ZV_k''} \right)^n \frac{k^{2n}}{p^{2n}} p_{\mu_1} ... p_{\mu_{2n}} \pi^{\mu_1}_{a_1} ... \pi^{\mu_{2n}}_{a_{2n}} \delta^{a_1 a_2} ... \delta^{a_{2n-1} a_{2n}} \right)$$

and utilizes the relation

$$\int_p^{\text{sym}} \frac{p_{\mu_1} ... p_{\mu_{2n}}}{p^{2n}} = \int_p^{\text{sym}} \frac{1}{c\,(n,d)} \left(\delta_{\mu_1 \mu_2} \; ... \; \delta_{\mu_{2n-1} \mu_{2n}} \; + \; \text{permutations} \right) \tag{4.47}$$

$$c(n,d) = \prod_{i=0}^{n-1} (d + 2i) = 2^n \frac{\Gamma[d/2 + n]}{\Gamma[d/2]} \tag{4.48}$$

for symmetric integrals. The r.h.s. of (4.47) consists of all permutations in μ_i modulo the identities $\delta_{\mu_1 \mu_2} = \delta_{\mu_2 \mu_1}$. However, all permutations apart from the first, depicted one lead to combinations of the momenta in (4.46) which cannot be expressed in terms Z and are hence not considered in the truncation. The coefficient $c(n,d)$ depends on the order n of the expansion and the spacetime dimension d and was determined by a combinatorical analysis based on the multiplication of both sides of (4.47) with $\delta^{\mu_1 \mu_2} \; ... \; \delta^{\mu_{2n-1} \mu_{2n}}$ which has to yield the integrand 1.
Evaluating the integral by means of the same analytic continuation as before, the result for $\dot{V}_k(Z)$ finally reads

$$\dot{V}_k(Z) = \frac{k^d}{(4\pi)^{d/2} \Gamma[d/2+1]} \left(\frac{(N-1)k^2}{4ZV_k'^2 - k^2} \right. \tag{4.49}$$
$$\left. + \sum_{n=1}^{\infty} \frac{(-1)^n k^{2n} 4ZV_k'^2}{(4ZV_k'^2 - k^2)^{n+1}} \left(\frac{V_k''}{V_k' + 2ZV_k''} \right)^n \frac{2^{-n} \Gamma[d/2]}{\Gamma[d/2 + n]} (2Z)^n \right)$$

This flow equation for a generic momentum potential can now be studied more explicitly by applying different ansätze for $V_k(Z)$. A natural choice is a polynomial series

$$V(Z) = \sum_{i=1}^{s} g_i Z^i \,, \tag{4.50}$$

in which the scale index was suppressed, as it will be in remainder of this chapter. It should be stressed that an expansion in higher than quadratic orders in the momenta is different from an expansion in order of derivatives, since the relation $\pi \propto \partial \phi$ no longer holds true.
The beta functions of g_m can be computed from (4.49) by taking m derivatives w.r.t. Z and subsequently evaluating at $Z = 0$. This can be done without too much effort

despite the appearance of an infinite sum in (4.49), because all but the first $m-1$ terms in the sum are of higher order in Z and do not contribute to the running of g_m. A systematic analysis with increasing order s of the truncation could thus be performed:
The renormalization of g_m is determined only by the couplings g_l with $l < m$. This immediately follows from the structure of (4.49). As an example, the first three (dimensionless) beta functions shall be stated here:

$$\begin{aligned}
\beta_{g_1} &= g_1 - \frac{2(N-1)}{3\pi^2} g_1^2 \\
\beta_{g_2} &= 5g_2 - \frac{8(N-1)}{3\pi^2} g_1^4 - \frac{8(3N-2)}{9\pi^2} g_1 g_2 \\
\beta_{g_3} &= 9g_3 - \frac{32(N-1)}{3\pi^2} g_1^6 - \frac{64(3N-2)}{9\pi^2} g_1^3 g_2 - \frac{8(5N-7)}{15\pi^2} g_2^2 - \frac{4(3N-1)}{3\pi^2} g_1 g_3
\end{aligned} \tag{4.51}$$

For each order of the truncation there are two fixed points: the trivial one with $g_m = 0$ for all m and a nontrivial one, at which the couplings g_m assume finite, positive values for $N \geq 3$. The example $s = 3$ reads

$$g_1^* = \frac{3\pi^2}{2(N-1)}\,, \; g_2^* = \frac{81\pi^6}{2(N-1)^2(3N-7)}\,, \; g_3^* = \frac{243\pi^{10}(585N^2 - 1722N + 1057)}{10(N-1)^4(3N-7)^3}\,.$$

The nontrivial fixed point has (for $N \geq 3$) only one IR-relevant direction in accordance with the general expectation and with the investigations in Chap. 3. The critical exponents corresponding to the irrelevant directions depend on N, but not the exponent Θ^R of the relevant direction which is the inverse of the critical exponent ν. Instead of a N-dependent ν, the AEHA computation yields the $N \to \infty$ value $\nu = 1$ for all N. This is the result of the simplest truncation and it cannot be improved, since the higher couplings have no impact on β_{g_1}. In case of the example $s = 3$ the critical exponents of the renormalization flow are

$$\left(1\,, \; -1 + \frac{4}{3(N-1)}\,, \; -3 + \frac{4}{N-1}\right)\,. \tag{4.52}$$

The higher orders in Z are irrelevant and will hence vanish in the IR description of the theory. This agrees with the successful use of quadratic actions like (4.42) or (2.1) as effective theories for low energies. If one investigates the renormalization properties starting from such scale of an effective, quadratic theory and employing the Hamiltonian formalism[8], one finds a nontrivial fixed point in the UV at each

[8]The covariant version of the Hamiltonian can be introduced at this scale without problems due to its quadratic structure.

order of the truncation, which indicates the non-perturbative renormalizability of the model. The corresponding fundamental theory seems to be more than quadratic in the momenta[9].

One may wonder if the non-quadratic structure of the UV theory is compatible with the regularization procedure. The longitudinal modes are properly regularized by the cutoff action, which provides the constraint $\delta(p_\mu(\varpi - \pi)^\mu)$ for $k \to \infty$. But while the coincidence limit $\varpi^\mu \to \pi^\mu$ is effectively given for the transverse modes as well in case of a quadratic Hamiltonian, it is very unlikely that a similar behavior also holds true for bare Hamiltonians of higher orders. A solution to this problem could be the elimination of the redundancy which was introduced by the enlargement of phase space by restricting the whole analysis to longitudinal modes only. This could be formally implemented by introducing the constraint $\delta(\Pi_\perp^{\mu\nu}\varpi_\nu)$ with $\Pi_\perp^{\mu\nu} = \mathbb{1} - \frac{p^\mu p^\nu}{p^2}$ into the path integral. Such a projection maintains the Lorentz-covariance of the computation, but breaks the reparametrization invariance. This invariance, however, is already broken by working in a specific choice of coordinates. If one applies this idea, the calculations proceed in the same way as outlined above up to Eq. (4.45). As $\pi_\mu \propto p_\mu$, the flow equation would simplify at this point to

$$\mathrm{i}\dot{V}(Z) = \int_p \Theta(k^2 - p^2) \left(\frac{(N-2)\, k^2}{4ZV'^2 - k^2} - 1 + \frac{4ZV'^2}{4ZV'^2 - k^2 \frac{V'}{V'+2ZV''}} \right) . \tag{4.53}$$

The resulting beta functions and the fixed point structure are almost the same as above and differ only by the numerical values of c_1, c_2 in the factors of the kind $(c_1 N - c_2)$. The existence of a nontrivial fixed point at each order of the truncation remains true and Θ^R is still 1, i.e. $\nu = 1$, for all N, while the remaining exponents increase with N.

4.4. Conclusions

The aim of this chapter was to explore if the "Hamiltonian point of view" on quantum field theories and nonlinear sigma models in particular can provide some additional insights. The analysis of the path integral measure (as well as the UV-asymptotics of the cutoff action) suggests that the standard flow equation of the FRG ought to be complemented by an additional regulator-dependent term. Possible consequences of such a modification were considered for the covariant analysis of nonlinear O(N) models which was performed in Chap. 3. A stabilization

[9] This finding is not equivalent, but similar to the result that the nontrivial fixed point which was found in Chap. 3 contains derivative operators of more than quadratic order.

of the fourth-order computations could be found, which supports the relevance of these measure corrections. However, the results for the critical exponent ν deviate strongly from the literature values, and in order to draw a decisive conclusion a more refined analysis of the measure is required for theories which are formulated in terms of a background field expansion.
The main part of the chapter was then devoted to the recently proposed Average Effective Hamiltonian Action approach, which is a Hamiltonian formulation of the FRG. First, a brief introduction to the AEHA and a derivation of the corresponding flow equation were presented, before the consistency of this approach with the standard Lagrangian FRG was shown by its application to simple truncations of linear and nonlinear sigma models. The interesting property of the Hamiltonian formulation is the possibility to investigate an alternative expansion of the truncation. The nonlinear O(N) models, in which operators of higher order in the momenta are naturally generated, were therefore studied as a test case. Using stereographic coordinates, the flow equation for a generic function $V(Z)$ of the expression $Z = \frac{1}{2}h^{ab}(\phi)\pi_a^\mu \pi_{b,\mu}$ was derived. Employing a polynomial ansatz for $V(Z)$ a fixed point with only one IR-relevant direction could be found in three dimensions for each N at every order of the truncation. While the approach is very stable, it is not sensitive to the nontrivial critical properties of the model which are encoded in $\nu(N)$. Although the exponents corresponding to the irrelevant directions depend on N, the one corresponding to the relevant direction yields the $N \to \infty$ result 1 for all N. At the end, a possible restriction of the analysis to longitudinal momentum modes was briefly discussed and a qualitative agreement with the previous results was found.

5. Renormalization of the CP^1 Model with Topological Term

The investigations presented in this chapter have already been published in [112].

One of the most interesting characteristics of the two-dimensional $O(3) \cong CP^1$ model, introduced in Sec. 2.3, is the nontrivial topology of the target space which allows for instantons and the definition of a topological charge Q, given in (2.16), that represents the winding number of the field configurations. The winding number labels distinct topological sectors of the configuration space and hence enables a weighting of these in the path integral by adding the term $i\theta Q$ to the (Euclidean) action[1]. The inclusion of such a θ-term in the action has attracted much attention since Haldane showed that antiferromagnetic spin-S chains can be mapped onto the O(3) model with $\theta = 2\pi S$ [113]. The physical properties of the model depend nontrivially on the topological parameter, most prominently the mass gap which vanishes for $\theta = \pi$ [114]. Furthermore, the vacuum energy density is a function of θ which can be seen in a large-N expansion as well as a dilute instanton gas approximation, cf. [115] and references therein. This θ-dependence of the mass gap and vacuum energy are also confirmed by numerical simulations, see e.g. [116] and [117]. More information about lattice computations of the sigma model with topological term are given in [118]. More recently, the case θ slightly below π was considered as a toy model for walking technicolor [119, 120].
Since the winding number is not altered by fluctuations, one would naively expect that this topological operator is not renormalized. In addition, it was explicitly shown in [117, 120] that since the topological charge distinguishes between different vacua, it cannot be an irrelevant operator that renormalizes to zero. On the other hand, the investigation of non-Abelian gauge theories, which share interesting properties with the sigma model, indicated that a finite renormalization of the θ-parameter occurs in the extreme momentum ranges. These nontrivial effects were first studied in [25, 26] and [27], and subsequently also by means of the Functional

[1] In Minkowski spacetime the additional term in the action simply reads θQ.

Renormalization Group (FRG) [28]. The result of the latter investigation was a finite, discrete renormalization of θ in the extreme UV and the extreme IR. A similar behavior in the extreme IR was found in an analysis of the coupling of Chern-Simons theory [29].

The purpose of this chapter is to examine by means of the FRG formalism if a similar renormalization of the topological parameter also occurs in nonlinear sigma models. The analysis will follow [28] and investigate a more general class of operators by considering a spacetime-dependent coupling $\theta \to \theta\alpha(x)$, where α is an auxiliary scalar field. The case $\alpha(x) = 1$ will be evaluated at the end. In order to perform a reparametrization invariant investigation, the topological operator (2.16) ought to be considered in its covariant formulation

$$Q[\phi] = \frac{1}{2\pi} \int d^2x \, \epsilon^{\mu\nu} \sqrt{h} \epsilon_{ab} \, \partial_\mu \phi^a \partial_\nu \phi^b \,, \tag{5.1}$$

where $h = \det h_{ab}$. It is reasonable to start the analysis with a simple ansatz for the EAA which consists only of the operators of the bare action, assuming that these are the dominant ones. If one takes the auxiliary field $\alpha(x)$ into account, the ansatz reads

$$\Gamma_k[\phi] = \frac{1}{2} \zeta_k \int d^2x \; h_{ab}(\phi) \partial_\mu \phi^a \partial^\mu \phi^b + \frac{\mathrm{i}}{2\pi} \theta_k \int d^2x \, \epsilon^{\mu\nu} \sqrt{h} \epsilon_{ab} \; \alpha \; \partial_\mu \phi^a \partial_\nu \phi^b \,, \tag{5.2}$$

A covariant formulation of the flow equation of the model will be derived in the next section, before the renormalization of the coupling ζ is discussed in Sec. 5.2. Thereafter the renormalization of θ is analyzed, first in the UV (Sec. 5.3) and subsequently in the IR (Sec. 5.4). The former will rely on an off-diagonal heat kernel expansion and the latter on a "fermionic" reformulation of the flow equation and an application of the index theorem. Since these computations do not commute with $\alpha(x) \to 1$, it should be kept in mind that the results of this analysis only hold true if one regards the topological term as the limit of such a more general operator.

5.1. Topological Terms in the FRG

The geometrical properties of nonlinear $\mathrm{O}(N)$ models, the covariant background field method and its application in the FRG formalism were already discussed in much detail in Sec. 3.2. Analogous to the standard action functional, the topological term (5.1) can be expanded in powers of fluctuations ξ about the background φ according to (3.9), by utilizing an affine parametrization $\varphi_\lambda, \lambda \in [0, 1]$ of the geodesic which connects φ with the full field ϕ:

$$Q[\phi] = \sum_{n\geq 0} \frac{1}{n!} \frac{d^n}{d\lambda^n} Q[\varphi_\lambda]\bigg|_{\lambda=0} = \sum_{n\geq 0} \frac{1}{n!} \nabla_\lambda^n Q[\varphi_\lambda]\bigg|_{\lambda=0} . \tag{5.3}$$

Owing to the one-loop structure of the flow equation (3.14), the renormalization of the single-field action functional is driven by the second order in the fluctuations ξ, which is in case of the topological charge

$$Q[\varphi, \xi]|_{\xi^2} = \frac{1}{2\pi} \int d^2x \, \epsilon^{\mu\nu} \sqrt{h} \epsilon_{ab} \, \alpha \left(\nabla_\mu \xi^a \nabla_\nu \xi^b + R^a{}_{cde} \partial_\mu \varphi^e \partial_\nu \varphi^b \xi^c \xi^d \right) . \tag{5.4}$$

Again, the covariant derivative as well as the metric and the Riemann tensor have to be understood as evaluated at the base-point φ. Taking into account the commutator of the pullback derivatives (2.8) and using the first Bianchi identity, one can calculate the second derivative w.r.t. ξ , evaluated at the base-point $\phi = \varphi$:

$$Q_{ab}^{(0,2)}[\varphi, 0] = -\frac{1}{\pi} \epsilon^{\mu\nu} (\partial_\mu \alpha) \sqrt{h} \epsilon_{ac} \nabla^c_{\nu,b} . \tag{5.5}$$

This result shows that the flow equation is sensitive to the topological term, only if it is considered in a generalized form which contains a spacetime-dependent auxiliary field. It follows

$$\begin{aligned} \Gamma^{(0,2)}_{k,ab}[\varphi, 0] &= -\zeta_k (\nabla_\mu \nabla^\mu)_{ab} + \zeta_k \underbrace{R_{acdb} \partial_\mu \varphi^c \partial^\mu \varphi^d}_{=M_{ab}} - \underbrace{\frac{\mathrm{i}}{\pi} \theta_k \, \epsilon^{\mu\nu} (\partial_\mu \alpha) \sqrt{h} \epsilon_{ac} \nabla^c_{\nu,b}}_{=B_{ab}(\alpha)} \\ &= \zeta_k \, \tilde{\Delta}_{ab} - B_{ab}(\alpha) . \end{aligned} \tag{5.6}$$

As the physical properties of the system should be independent of the specific regularization scheme, there is some freedom to choose an appropriate regulator $\mathcal{R}_k$. A reasonable choice with regard to the following computations is a coarse-graining with respect to the Laplacian operator $\tilde{\Delta}_{ab} = -(\nabla_\mu \nabla^\mu)_{ab} + M_{ab}$. For the truncation studied here, a coarse-graining w.r.t. $\Delta_{ab} = -(\nabla_\mu \nabla^\mu)_{ab}$, for instance, would not change the discussion of the renormalization in the UV. In the IR, however, the choice $\tilde{\Delta}_{ab}$ becomes particularly useful, since it allows for an interesting reformulation of the problem, see Sec. 5.4.

In order to make the computations more transparent, it is furthermore convenient to rescale the regulator and extract a factor[2] ζ_k. The regulator thus reads

$$\mathcal{R}_k = \zeta_k R_k(\tilde{\Delta}) \qquad \Rightarrow \qquad \dot{\mathcal{R}}_k = \zeta_k\big(\dot{R}_k(\tilde{\Delta}) - \eta_\zeta R_k(\tilde{\Delta})\big) \;\text{ with }\; \eta_\zeta = -\frac{\dot{\zeta}_k}{\zeta_k}\,. \tag{5.7}$$

In case a further specification of the regulator R_k is necessary in this chapter, the optimized regulator (2.34) will be used.
The beta functions, $\beta_\zeta = \dot{\zeta}_k$ and $\beta_\theta = \dot{\theta}_k$, can be determined by matching the corresponding operators on both sides of the flow equation, which is given in (3.14). As mentioned in Sec. 3.2, the only way to determine the renormalization of a covariant single-field functional is to evaluate the flow equation at $\phi = \varphi$, i.e. $\xi = 0$. This is also a convenient choice from a computational point of view and the l.h.s. of (3.14) simplifies to

$$\dot{\Gamma}_k[\varphi] = \frac{1}{2}\,\beta_\zeta \int d^2x\; h_{ab}(\varphi)\partial_\mu\varphi^a\partial^\mu\varphi^b + \frac{\mathrm{i}}{2\pi}\,\beta_\theta \int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b\,. \tag{5.8}$$

In order to project the r.h.s. of (3.14) onto these operators, an expansion in $B(\alpha)$ is employed which is justified for small fluctuations $\partial_\mu\alpha$ and leads to a separation of symmetric and antisymmetric tensors:

$$\begin{aligned}
\dot{\Gamma}_k &= \frac{1}{2}\mathrm{Tr}\left\{\frac{\zeta_k\big(\dot{R}_k(\tilde{\Delta}) - \eta_\zeta R_k(\tilde{\Delta})\big)}{\zeta_k R_k(\tilde{\Delta}) + \zeta_k\tilde{\Delta} - B(\alpha)}\right\} \\
&= \frac{1}{2}\mathrm{Tr}\left\{\underbrace{\frac{\dot{R}_k - \eta_\zeta R_k}{R_k + \tilde{\Delta}}} \;+\; \zeta_k^{-1}(\dot{R}_k - \eta_\zeta R_k)(R_k+\tilde{\Delta})^{-1}B(\alpha)(R_k+\tilde{\Delta})^{-1} + O(B^2)\right\} \\
&= \frac{1}{2}\mathrm{Tr}\Big\{\quad W(\tilde{\Delta}) \quad + \;\zeta_k^{-1}\,B(\alpha)\;f(\tilde{\Delta}) \;+\; \mathcal{O}(B^2)\Big\}\,.
\end{aligned} \tag{5.9}$$

The terms of order $\mathcal{O}(B^2)$ will be neglected in the following analysis. It was explicitly checked that they only yield terms of fourth or higher order in the derivatives which are not considered in the truncation.
The first term in (5.9) contains no antisymmetric tensor and hence does not contribute to the running of θ. It will be discussed first. The relevant contributions to β_θ are given by the second term and will be investigated in Sec. 5.3 and 5.4, where it will also become apparent that the second term does not contribute to the running of ζ.

[2] This rescaling is compatible with the required asymptotic behavior of the regulator owing to the well-established asymptotic freedom of the model with regard to the coupling $g = \zeta^{-1/2}$.

5.2. The Running of ζ

The renormalization of ζ is determined solely by the expression $\frac{1}{2}\mathrm{Tr}\{W(\tilde{\Delta})\}$, which can be calculated by means of a Laplace transform and a heat kernel expansion:

$$\frac{1}{2}\mathrm{Tr}\{W(\tilde{\Delta})\} = \frac{1}{2}\int_0^\infty ds\ \tilde{W}(s)\ \mathrm{Tr}\left\{\mathrm{e}^{-s\tilde{\Delta}}\right\} = \frac{1}{2}\int_0^\infty ds\ \tilde{W}(s)\ \frac{1}{4\pi s}\sum_{n=0}^{\infty} s^n c_n\,.$$

The first few coefficients of this heat kernel expansion are well-studied, cf. [121]. Only $c_1 = -\int_x M^a{}_a$, with M_{ab} defined in Eq. (5.6), affects the running of ζ, because all coefficients c_n with $n \geq 2$ are of higher orders in the derivatives, and c_0 simply yields a field-independent renormalization of the vacuum energy. The s-integration for $n = 1$ simplifies to $\int_0^\infty ds\ \tilde{W}(s) = W(0)$. For the optimized regulator given above, this expression is equal to $2-\eta_\zeta$. The trace of $-M_{ab}$ in target space yields $h_{ab}\,\partial_\mu\varphi^a\partial^\mu\varphi^b$, since $R_{abcd} = h_{ac}h_{bd} - h_{ad}h_{bc}$ on S^2, and one can relate both sides of the flow equation such that

$$\begin{aligned}\frac{1}{2}\,\beta_\zeta\int d^2x\ h_{ab}(\varphi)\partial_\mu\varphi^a\partial^\mu\varphi^b &= \frac{1}{8\pi}(2-\eta_\zeta)\int d^2x\ h_{ab}(\varphi)\partial_\mu\varphi^a\partial^\mu\varphi^b\\ \Rightarrow\ \beta_\zeta = \frac{1}{4\pi}(2-\eta_\zeta)\quad &\Leftrightarrow\quad \beta_\zeta = \frac{2\zeta_k}{4\pi\zeta_k - 1}\,.\end{aligned}\tag{5.10}$$

Note that g with $\zeta = g^{-2}$ is the usually studied coupling of the model and its beta function is

$$\beta_g = -\frac{1}{4\pi}\,g^3\left(1-\frac{g^2}{4\pi}\right)^{-1}\,.\tag{5.11}$$

This result confirms the well-known asymptotic freedom of the nonlinear sigma model in two dimensions [41]. The pole at $g^2 = 4\pi$ is only an unphysical artefact of the specific regulator choice (5.7). The beta functions (5.10) and (5.11) agree with previous computations within the FRG scheme [43], apart from an unimportant numerical factor which is due to a slightly different regularization.

Since the mass spectrum of the theory, i.e. the threshold in the flow equation, depends on θ, one should expect that also β_ζ is affected by this parameter. The beta function (5.10), however, is independent of θ, and higher orders in $B(\alpha)$ in the expansion (5.9) do not influence the running of ζ, either, but only yield antisymmetric tensors . The absence of a θ-dependence is not a shortcoming of the specific expansion. In an alternative treatment of the flow equation by means of a heat kernel expansion of a modified Laplacian, which incorporates the derivative operator $B(\alpha)$, β_ζ is also independent of θ.

A direct investigation of the mass spectrum of the nonlinear sigma model is difficult within the covariant FRG scheme employed here, since the introduction of a mass term for the full field ϕ or the background φ would break the reparametrization invariance. One could introduce a covariant mass term $m_k^2 h_{ab}(\varphi)\xi^a\xi^b$ for the fluctuations and compute its running in the way outlined in [79]. However, explicit calculations show that the flow of m_k^2 is not affected by θ_k, either. One has to conclude that the chosen ansatz for the effective action is apparently not sensitive to the nontrivial θ-dependence of the spectrum, and one ought to study larger truncations for this purpose.

5.3. Renormalization of θ in the UV

In order to evaluate the second term in (5.9), one can again apply a Laplace transform, $f(\tilde{\Delta}) = \int_0^\infty ds\, \tilde{f}(s)\, \exp\left(-s\tilde{\Delta}\right)$, and evaluate the action of $B(\alpha)$ on this expression by means of off-diagonal elements of a heat kernel expansion:

$$
\begin{aligned}
&\mathrm{Tr}\left\{\zeta_k^{-1} B(\alpha) f(\tilde{\Delta})\right\} &(5.12)\\
&= \frac{\mathrm{i}}{\pi}\frac{\theta_k}{\zeta_k}\int d^2x\, d^2y\, \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\int_0^\infty ds\, \tilde{f}(s)\, \underbrace{\langle x|\,(\partial_\mu\alpha)\nabla_\nu\,|y\rangle^{bc}}_{=\partial_\mu\alpha(x)\nabla_\nu(x)\delta(x-y)}\underbrace{\langle y|\,\mathrm{e}^{-s\tilde{\Delta}}\,|x\rangle_c^{\;a}}_{\equiv\Omega(y,x,s)}\\
&= -\frac{\mathrm{i}}{\pi}\frac{\theta_k}{\zeta_k}\int d^2x\, d^2y\, \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\int_0^\infty ds\, \tilde{f}(s)\ \alpha(x)\ \delta(x-y)\ \times\\
&\qquad\times\left(\frac{1}{2}H_{\mu\nu}(y)\Omega(y,x,s) + \nabla_\mu(x)\nabla_\nu(y)\Omega(y,x,s)\right)^{ba},
\end{aligned}
$$

where $H_{\mu\nu}$ is the commutator of the pullback derivatives introduces in (2.8). Following the reasoning that the limit $\alpha(x)\to 1$ is performed at the end, it is justified to neglect the surface terms coming from integration by parts. Since the infinitesimal separation of x and y regularizes the expression and provides access to nontrivial information about the UV, the δ-function $\delta(x-y)$ ought to be understood as limit $y\to x$ which has to be performed carefully.

In order to evaluate (5.12), appropriate expressions for the off-diagonal elements $\Omega(x,y,s)$ are required, which shall be derived here. Note that the indices of the target manifold will be suppressed for sake of brevity and that the following derivation applies for two dimensions, but could be generalized to other dimensions. Starting with the generic ansatz

$$\Omega(x,y,s) = \big\langle x\big|\mathrm{e}^{-s\tilde{\Delta}}\big|y\big\rangle = \frac{1}{4\pi s}\mathrm{e}^{-\frac{|x-y|^2}{4s}}\sum_{n=0}^{\infty} s^n c_n(x,y)\,, \tag{5.13}$$

the following constraint can be deduced from $\big(\frac{d}{ds}+\tilde{\Delta}_x\big)\Omega(x,y,s)=0$ for the coefficients $c_n(x,y)$:

$$n\,c_n + (x^\mu - y^\mu)\nabla_{x^\mu}\,c_n + \tilde{\Delta}_x\,c_{n-1} = 0\,. \tag{5.14}$$

For $n=0$ the constraint simplifies to $(x^\mu - y^\mu)\nabla_{x^\mu}c_0 = 0$ and is solved by

$$c_0(x,y) = \mathcal{P}\ \mathrm{e}^{-\int_y^x dz^\mu\,\Gamma\partial_\mu\varphi}\,, \tag{5.15}$$

where $\mathcal{P}$ denotes the ordering of the operators according to the path from y to x, which is understood to be a straight line here. The covariant derivative $\nabla_{x^\mu}c_0(x,y)$ was discussed in much detail, for instance, in (the appendix of) [122] for the case of a gauge field and the result can be transferred to the pullback connection $\Gamma\partial_\mu\varphi$ with little effort. It yields

$$\nabla_{x^\mu}\,c_0(x,y) = \int_0^1 dt\,t\,(x-y)^\rho\,c_0(x,z)\,H_{\rho\mu}(z)\,c_0(z,y) \quad \text{with } z = y+t(x-y)\,. \tag{5.16}$$

This expression can be expanded in different ways:

$$\begin{aligned}
&\nabla_{x^\mu}\,c_0(x,y) && (5.17)\\
&= -\frac{1}{2}c_0(x,y)H_{\mu\rho}(y)(x-y)^\rho + \frac{1}{3}c_0(x,y)\nabla_\sigma H_{\mu\rho}(y)\cdot(x-y)^\sigma(x-y)^\rho + O(x-y)^3\\
&= -\frac{1}{2}H_{\mu\rho}(x)(x-y)^\rho c_0(x,y) + \frac{1}{6}\nabla_\sigma H_{\mu\rho}(x)\cdot(x-y)^\sigma(x-y)^\rho c_0(x,y) + O(x-y)^3\,.
\end{aligned}$$

While Eq. (5.16) proves that $(x^\mu - y^\mu)\nabla_{x^\mu}c_0 = 0$ due to the antisymmetry of $H_{\rho\mu}$, especially the relations (5.17) will be relevant for the calculation of (5.12). Based on c_0, a recursive solution for the higher coefficients can be constructed as[3]

$$c_n(x,y) = -c_0(x,y)\int_0^1 d\lambda\ \lambda^{n-1}\Big(c_0^{-1}(x,y)\,\tilde{\Delta}\,c_{n-1}(x,y)\Big)^{*\lambda}\,. \tag{5.18}$$

[3] The expression is inspired by the solution to a similar problem in gauge theory [123], which is yet a bit simplier owing to the choice of a specific gauge.

The symbol $\big(A(x,y)\big)^{*\lambda}$ denotes an expansion[4] of some operator $A(x,y)$ about y in powers of $(x-y)^\mu$, in which each factor $(x-y)^\mu$ is multiplied by λ. Although this expression is rather abstract, it will be sufficient for the purposes of this investigation. Remembering that $(x^\mu - y^\mu)\nabla_{x^\mu} c_0 = 0$, it indeed provides the correct off-diagonal heat kernel coefficients:

$$
\begin{aligned}
(x^\mu - y^\mu)\nabla_{x^\mu} c_n &= -\, c_0 \int_0^1 d\lambda\ \lambda^{n-1}(x-y)^\mu \partial_{x^\mu} \left(c_0^{-1}\tilde{\Delta}\, c_{n-1}\right)^{*\lambda} \\
&= -\, c_0 \int_0^1 d\lambda\ \lambda^{n-1}\lambda \frac{\partial}{\partial\lambda} \left(c_0^{-1}\tilde{\Delta}\, c_{n-1}\right)^{*\lambda} \\
&= -\, c_0 \left[\lambda^n \left(c_0^{-1}\tilde{\Delta}\, c_{n-1}\right)^{*\lambda}\right]_{\lambda=0}^{\lambda=1} + n\, c_0 \int_0^1 d\lambda\ \lambda^{n-1} \left(c_0^{-1}\tilde{\Delta}\, c_{n-1}\right)^{*\lambda} \\
&= \ -\tilde{\Delta}\, c_{n-1} - n\, c_n\,.
\end{aligned} \tag{5.19}
$$

Based on this expansion of $\Omega(x,y,s)$ one can evaluate the trace (5.12). According to (5.18), all c_n with $n \geq 1$ are of second or higher order in the derivatives, such that the action of $\nabla_\mu(y)\nabla_\nu(x)$ on these coefficients yields only terms of fourth or higher order in the derivatives which are not considered in our truncation. The derivatives of c_0 are given in (5.17). Applying them in (5.12) yields

$$
\begin{aligned}
&\mathrm{Tr}\left\{\zeta_k^{-1} B(\alpha) f(\tilde{\Delta})\right\} \qquad\qquad (5.20)\\
&= -\frac{\mathrm{i}}{\pi}\frac{\theta_k}{\zeta_k} \int d^2x \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\ \alpha(x) \lim_{y\to x} \int_0^\infty ds\ \tilde{f}(s) \frac{1}{4\pi s}\left(\frac{1}{2}H_{\mu\nu}(x) + \delta_{\mu\nu}\frac{1}{2s}\right. \\
&\quad \left. - \frac{1}{4s^2}(x-y)_\mu(x-y)_\nu + \frac{(x-y)_\nu}{2s} H_{\mu\rho}(x)(x-y)^\rho + \frac{1}{2}H_{\nu\mu}(x)\right)_c^b \mathrm{e}^{-\frac{|x-y|^2}{4s}} c_0^{ca}(x,y) + \mathcal{O}(\partial\varphi)^3 \\
&= -\frac{\mathrm{i}}{\pi}\frac{\theta_k}{\zeta_k} \int d^2x\, \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\, \alpha \lim_{y\to x} \int_0^\infty ds\, \tilde{f}(s)\, \frac{1}{8\pi s^2}\, \mathrm{e}^{-\frac{|x-y|^2}{4s}} \times \\
&\qquad\qquad \times H_{\mu\rho}^{bc}(x)(x-y)^\rho(x-y)_\nu\ (c_0)_c{}^a(x,y) + \mathcal{O}\big((\partial\varphi)^3\big)\,.
\end{aligned}
$$

The function $c_0(x,y) = \mathrm{e}^{-\int_y^x \Gamma\partial\varphi\, dx'}$ of the pullback connection can be regarded as the identity in the further calculations, as the higher orders in the corresponding series only lead to terms which are beyond the chosen truncation. The tensor $\epsilon_{ab}H_{\mu\rho}^{ba}$ is equal to $-2\epsilon_{ab}\partial_\mu\varphi^a\partial_\rho\varphi^b$, taking into account that $H_{\mu\rho}^{ba} = R^{ba}{}_{cd}\partial_\mu\varphi^c\partial_\rho\varphi^d$ and that for a sphere $R_{abcd} = h_{ac}h_{bd} - h_{ad}h_{bc}$. In two dimensions the Lorentz indices can be

[4] Owing to the recursive construction, the coefficient c_n is expandable about y in powers of $(x-y)^\mu$ as long as c_{n-1} is, and because c_0 is expandable, this holds true for all c_n.

rearranged as follows

$$\begin{aligned}\epsilon_{ab}\,\epsilon^{\mu\nu}\,\partial_\mu\varphi^a\partial_\rho\varphi^b\,(x-y)^\rho\,(x-y)_\nu &= \epsilon_{ab}\,\partial_1\varphi^a\partial_2\varphi^b(x-y)_2^2 - \epsilon_{ab}\,\partial_2\varphi^a\partial_1\varphi^b(x-y)_1^2 \\ &= \frac{1}{2}\epsilon_{ab}\,\epsilon^{\mu\nu}\,\partial_\mu\varphi^a\partial_\nu\varphi^b(x-y)^2\,. \end{aligned} \tag{5.21}$$

The renormalization of the topological parameter θ can now be determined by a comparison of (5.20) with the l.h.s. of the flow equation as it is given in Eq. (5.8):

$$\begin{aligned} &\frac{\mathrm{i}}{2\pi}\,\beta_\theta \int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b \\ &\qquad = \frac{\mathrm{i}}{2\pi}\,\frac{\theta_k}{\zeta_k}\int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\lim_{y\to x}\int_0^\infty ds\;\tilde{f}(s)\frac{(x-y)^2}{8\pi s^2}\mathrm{e}^{-\frac{|x-y|^2}{4s}}\,\partial_\mu\varphi^a\partial_\nu\varphi^b \\ &\Longrightarrow\;\; \beta_\theta = \frac{\theta_k}{\zeta_k}\,\lim_{u\to 0}\int_0^\infty ds\;\tilde{f}(s)\,\frac{u^2}{8\pi s^2}\;\mathrm{e}^{-\frac{u^2}{4s}}\,. \end{aligned} \tag{5.22}$$

This beta function vanishes for any finite value of s in the limit $u \to 0$. In order to analyze if the limit $s \to 0$ yields relevant contributions, it is useful to notice that the inverse Laplace transform $\tilde{f}(s)$ is in fact a function of $k^2 s$ which can be denoted by $\sigma(k^2 s)$:

$$\sigma(k^2 s) = \mathcal{L}^{-1}\left[\frac{\dot{R}_k(z) - \eta_k R_k(z)}{\big(z + R_k(z)\big)^2}\right](s) \tag{5.23}$$

$$= -\mathcal{L}^{-1}\Big[k\partial_k\big(z + R_k(z)\big)^{-1}\Big](s) - \mathcal{L}^{-1}\left[\frac{\eta_k\,R_k(z)}{\big(z + R_k(z)\big)^2}\right](s) \equiv -k\partial_k\,\sigma_1(k^2 s) - \eta_k\,\sigma_2(k^2 s)\,.$$

This can be understood if one considers the Laplace transform at $k = 1$, rescales with $z \to z/k^2$ and remembers that the structure of the regulator is $z \cdot r(z/k^2)$ for dimensional reasons. The case σ_1, for instance, reads

$$\begin{aligned} &\big(z + R_{k=1}(z)\big)^{-1} = \int_0^\infty ds\;\sigma_1(s)\,\mathrm{e}^{-sz} \\ &\Rightarrow\;\; k^2\big(z + R_k(z)\big)^{-1} = \int_0^\infty ds\;\sigma_1(s)\,\mathrm{e}^{-s\frac{z}{k^2}} = \int_0^\infty ds'\;k^2\sigma_1(k^2 s')\,\mathrm{e}^{-s'z}\,. \end{aligned} \tag{5.24}$$

The limit $s \to 0$ can be probed in a controlled way, if one integrates $\beta_\theta = 2\,k^2\partial_{k^2}\theta$ from the extreme UV down to some finite k_0 and applies two substitutions, first

$s \to \frac{1}{4}u^2 s$ and then $p^2 \equiv \frac{1}{4}u^2k^2s$:

$$\theta(\infty) - \theta(k_0^2) = \int_{k_0^2}^{\infty} dk^2 \lim_{u\to 0}\int_0^\infty ds\,\frac{u^2}{8\pi s^2}\,\mathrm{e}^{-\frac{u^2}{4s}}\left[-\partial_{k^2}\,\sigma_1(k^2 s) - \eta_k\,\frac{1}{2k^2}\,\sigma_2(k^2 s)\right]\frac{\theta}{\zeta}(k^2)$$
$$= -\lim_{u\to 0}\int_0^\infty ds\,\frac{1}{2\pi s^2}\,\mathrm{e}^{-\frac{1}{s}}\int_{k_0^2}^\infty dk^2\,\left[\partial_{k^2}\,\sigma_1\left(\frac{1}{4}u^2k^2s\right) + \eta_k\,\frac{1}{2k^2}\,\sigma_2\left(\frac{1}{4}u^2k^2s\right)\right]\frac{\theta}{\zeta}(k^2)$$
$$= -\int_0^\infty ds\,\frac{1}{2\pi s^2}\,\mathrm{e}^{-\frac{1}{s}}\lim_{u\to 0}\int_{\frac{1}{4}k_0^2\,u^2 s}^\infty dp^2\,\left[\partial_{p^2}\sigma_1(p^2)\,\frac{\theta}{\zeta}\left(\frac{4p^2}{u^2 s}\right) + \frac{1}{2p^2}\sigma_2(p^2)\,\eta\left(\frac{4p^2}{u^2 s}\right)\frac{\theta}{\zeta}\left(\frac{4p^2}{u^2 s}\right)\right]$$

The limit $u \to 0$ can be performed, while the s-integration remains finite and simply yields $\frac{1}{2\pi}$. The result is

$$\theta(\infty) - \theta(k_0^2) = \frac{1}{2\pi}\int_0^\infty dp^2\,\left[-\partial_{p^2}\sigma_1(p^2)\,\frac{\theta}{\zeta}(\infty) - \frac{1}{2p^2}\sigma_2(p^2)\,\eta(\infty)\,\frac{\theta}{\zeta}(\infty)\right]. \tag{5.25}$$

The p^2-integration is finite for an appropriate choice of regulator[5]. The renormalization of θ down to any finite scale k_0 obviously depends only on the values of θ, ζ and $\dot\zeta$ in the extreme UV and is formally given by a discrete "jump" at $k = \infty$. However, it is well-known and was confirmed in Sec. 5.2 that the theory is asymptotically free. This statement refers to the coupling $g = \zeta^{-1/2}$, which means that ζ diverges in the UV. The corresponding beta function, in contrast, remains finite for $\zeta \to \infty$, as given in (5.10). As a result, there is in fact no renormalization of the topological term at any finite k, as long as the bare coupling θ_∞ does not diverge:

$$\theta_k = \theta_\infty \quad \text{for any } k > 0\,. \tag{5.26}$$

This finding agrees with the usual expectation that the topological charge is not renormalized. However, the argumentation given above holds true only for finite k_0, but cannot be extended to $k = 0$. A careful investigation of the extreme IR and the zero modes is additionally required and will be given in the following chapter.
If one compares the analysis presented above with the one in [28], the structural similarities between Yang-Mills theory and the nonlinear sigma model are, once more, remarkable. According to [28], the renormalization of the topological charge in Yang-Mills theories is restricted for $k > 0$ to a jump in the extreme UV, similar to (5.25). However, taking the asymptotic freedom of the theory into account (i.e. $\bar g \to 0$) as it was done here, this jump vanishes as well.

[5]For instance, $\int_0^\infty s^{-1}\sigma_2(s)\,ds = \int_0^\infty dz\; R_{k=1}(z)[z + R_{k=1}(z)]^{-2}$.

5.4. Renormalization of θ in the IR

In Yang-Mills theory the investigation of the topological parameter in the IR [28] is based on a reformulation of a four-dimensional problem in terms of an eight-dimensional representation of the Clifford algebra [27] which relies on the 't Hooft symbol $\eta_{\alpha\beta\nu}$ [124]. A similar reformulation in a "fermionic language" is possible in case of the nonlinear sigma model and allows to study the zero modes. However, since there is no 't Hooft symbol available, one first has to develop a suitable representation of the Clifford algebra.

Consider a four-dimensional representation of the Gamma matrices Γ_μ which is based on two-dimensional matrices Ω_μ as follows

$$\Gamma_\mu \equiv \begin{bmatrix} 0 & \Omega_\mu \\ \Omega_\mu^\mathsf{T} & 0 \end{bmatrix} \quad \text{with} \quad \Omega_1 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \epsilon^a{}_b\,, \quad \Omega_2 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \delta^a{}_b\,. \tag{5.27}$$

Note that this construction does not introduce additional spinorial degrees of freedom, but is built upon the symmetric and the antisymmetric tensor in the tanget space of the model. The Γ_μ are defined on the tensor product of the tangent space with itself. The identities

$$\Omega_\mu \Omega_\nu^\mathsf{T} = \delta_{\mu\nu}\delta^a{}_b + \epsilon_{\mu\nu}\epsilon^a{}_b \qquad \Omega_\mu^\mathsf{T}\Omega_\nu = \delta_{\mu\nu}\delta^a{}_b - \epsilon_{\mu\nu}\epsilon^a{}_b \tag{5.28}$$

$$\Rightarrow \quad \Omega_\mu\Omega_\nu^\mathsf{T} + \Omega_\nu\Omega_\mu^\mathsf{T} = \Omega_\mu^\mathsf{T}\Omega_\nu + \Omega_\nu^\mathsf{T}\Omega_\mu = 2\delta_{\mu\nu}\delta^a{}_b \qquad \Omega_\mu\Omega_\nu^\mathsf{T} - \Omega_\mu^\mathsf{T}\Omega_\nu = 2\epsilon_{\mu\nu}\epsilon^a{}_b$$

will become useful and ensure the algebraic relation

$$\left\{\Gamma_\mu, \Gamma_\nu\right\} = \begin{bmatrix} \Omega_\mu\Omega_\nu^\mathsf{T} + \Omega_\nu\Omega_\mu^\mathsf{T} & 0 \\ 0 & \Omega_\nu^\mathsf{T}\Omega_\mu + \Omega_\nu^\mathsf{T}\Omega_\mu \end{bmatrix} = 2\delta_{\mu\nu}\mathbb{1}_4\,. \tag{5.29}$$

Moreover, one can define the gamma matrix Γ_*,

$$\Gamma_* = -\begin{bmatrix} \epsilon^a{}_b & 0 \\ 0 & \epsilon^a{}_b \end{bmatrix}\Gamma_1\Gamma_2 = \begin{bmatrix} -\epsilon^a{}_b\Omega_1\Omega_2^\mathsf{T} & 0 \\ 0 & -\epsilon^a{}_b\Omega_1^\mathsf{T}\Omega_2 \end{bmatrix} = \begin{bmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{bmatrix}, \tag{5.30}$$

$$\left\{\Gamma_*, \Gamma_\mu\right\} = 0\,, \quad \Gamma_*^2 = \mathbb{1}_4\,, \tag{5.31}$$

which provides a notion of chirality. In the following computations the Dirac operators

$$\not{D} \equiv \Gamma_\mu\nabla^\mu, \quad D \equiv \Omega_\mu\nabla^\mu, \text{ and } D^\mathsf{T} \equiv \Omega_\mu^\mathsf{T}\nabla^\mu \tag{5.32}$$

will be of particular importance and one may wonder if these expressions are well-defined, since the connection $\Gamma^a{}_{cb}\partial_\mu\varphi^c$ acts on the same space as the gamma matrices. However, both objects are simply linear combinations of $\epsilon^a{}_b$ and $\delta^a{}_b$ and hence commute with each other.

By means of these Dirac operators the flow equation can be rewritten. According to (5.9), the running of θ is determined by:

$$\begin{aligned}\frac{\mathrm{i}}{2\pi}\,\beta_\theta\int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b &= \frac{\mathrm{i}}{2\pi}\frac{\theta_k}{\zeta_k}\int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\partial_\mu\alpha(x)\big\langle x|\nabla_\nu f(\tilde{\Delta})|x\big\rangle^{ba}\\ &= \frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\;\partial_\mu\alpha(x)\,\mathrm{tr}_2\Big\{\big\langle x|(\Omega^\mu D^\intercal-\Omega^{\mu\intercal}D)f(\tilde{\Delta})|x\big\rangle\Big\}\,,\end{aligned}\tag{5.33}$$

where tr_2 denotes the trace in the two-dimensional tangent space of the model. The flow equation holds true for each field configuration and it can hence be evaluated at a configuration which is convenient from a computational point of view. In the present case self-dual fields are a particular useful choice, i.e. fields for which $\partial^\mu\varphi_a = \epsilon^{\mu\rho}\,\epsilon_{ab}\,\partial_\rho\varphi^b$. Remembering that $R_{abcd} = h_{ac}h_{bd} - h_{ad}h_{bc}$ and $[\nabla_\mu,\nabla_\nu]_{ab} = R_{abcd}\partial_\mu\varphi^c\partial_\nu\varphi^d$, it is easy to check that for self-dual fields

$$\begin{aligned}&M_{ab} = \epsilon^{\mu\nu}\epsilon_{ac}(\nabla_\mu\nabla_\nu)^c{}_b\,,\\ &\tilde{\Delta}_{ab} = -D^\intercal D\,,\quad \tilde{\Delta}_{ab} - 2M_{ab} = -DD^\intercal\,.\end{aligned}\tag{5.34}$$

With these relations the r.h.s. of (5.33) can be written as

$$\begin{aligned}&\frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\;\partial_\mu\alpha(x)\,\mathrm{tr}_2\left\{\langle x|\,(\Omega^\mu D^\intercal-\Omega^{\mu\intercal}D)f(-D^\intercal D)\,|x\rangle\right\}\\ &=\frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\;\partial_\mu\alpha(x)\,\mathrm{tr}_2\left\{\langle x|\,\Omega^\mu D^\intercal f(-DD^\intercal)-\Omega^{\mu\intercal}D\,f(-D^\intercal D)\right.\\ &\qquad\qquad\left.-\Omega^\mu D^\intercal\big(f(-DD^\intercal)-f(-D^\intercal D)\big)\,|x\rangle\right\}\,.\end{aligned}\tag{5.35}$$

The last term in (5.35) is of order $\mathcal{O}\big((\partial\varphi)^3\big)$ and can be neglected, since $f(-DD^\intercal)$ and $f(-D^\intercal D)$ differ only in terms of second order in the derivatives. The two-dimensional trace can now be expressed by means of the gamma matrices as a four-dimensional trace:

$$
\begin{aligned}
&\frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\; \partial_\mu\alpha(x)\,\mathrm{tr}_2\big\{\langle x|\Omega^\mu D^\intercal f(-DD^\intercal) - \Omega^{\mu\intercal} D\, f(-D^\intercal D)|x\rangle\big\}\\
&= \frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\; \partial_\mu\alpha(x)\,\mathrm{tr}_4\left\{\langle x|\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\Omega^\mu D^\intercal & 0\\ 0 & \Omega^{\mu\intercal} D\end{bmatrix} f\left(\begin{bmatrix}-DD^\intercal & 0\\ 0 & -D^\intercal D\end{bmatrix}\right)|x\rangle\right\}\\
&= \frac{\mathrm{i}}{4\pi}\frac{\theta_k}{\zeta_k}\int d^2x\; \partial_\mu\alpha(x)\,\mathrm{tr}_4\left\{\langle x|\,\Gamma_*\Gamma^\mu \not{D} f(-\not{D}^2)|x\rangle\right\}\,. \qquad (5.36)
\end{aligned}
$$

In the IR regime the trace is well-defined due to the presence of the regulator and one can integrate by parts[6] in order to shift the derivative acting on $\alpha(x)$ to the trace. It acts on bra and ket vector separately and can be contracted[7] with Γ^μ. The resulting expression shows that only the zero modes provide a non-vanishing contribution:

$$
\frac{\mathrm{i}}{2\pi}\beta_\theta \int d^2x\, \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b = -\frac{\mathrm{i}}{2\pi}\frac{\theta_k}{\zeta_k}\int d^2x\;\alpha(x)\,\mathrm{tr}_4\left\{\langle x|\,\Gamma_*\not{D}^2 f(-\not{D}^2)|x\rangle\right\}\,. \qquad (5.37)
$$

The spectrum of $-\not{D}^2$ is degenerate and all non-zero-modes appear in pairs of opposite “chirality”, which cancel each other in the trace due to Γ_*. In order to determine the contribution of the zero modes, one can integrate the beta function (5.37) between $k = 0$ and a finite, but arbitrarily small k_0. Since $\dot{\zeta}$ is a continuous function (as confirmed in Sec. 5.2), it is a reasonable approximation to consider $\zeta_k = \zeta_0$ and $\dot{\zeta}_k = \dot{\zeta}_0$ in this infinitesimal momentum range. The renormalization of θ due to IR effects is hence given as

$$
\begin{aligned}
&(\theta_{k_0^2} - \theta_0)\int d^2x\, \epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b = \mathrm{Tr}_4\left\{\alpha\,\zeta_0^{-1}\Gamma_*\lim_{\lambda\to 0}\int_0^{k_0^2} dk^2\;\theta(k^2)\,\lambda f(\lambda)\right\}\\
&= \mathrm{Tr}_4\left\{\alpha\,\zeta_0^{-1}\Gamma_*\lim_{\lambda\to 0}\int_0^{k_0^2} dk^2\;\theta(k^2)\,\lambda\left(-\frac{d}{dk^2}[R_k(\lambda)+\lambda]^{-1} - \frac{1}{2k^2}\eta_{\zeta_0}\frac{R_k(\lambda)}{(R_k(\lambda)+\lambda)^2}\right)\right\}.
\end{aligned}
$$

---

[6] Assuming appropriate properties of $\alpha(x)$ such that the surface terms can be neglected. Remember that the limit $\alpha(x) \to 1$ is performed at the end.

[7] The matrix Γ^μ anticommutes with Γ_* and, utilizing the cyclicality of the trace, it can be contracted with the derivative acting on $|x\rangle$. The resulting $\not{D}$ then commutes with $\not{D} f(-\not{D}^2)$.

Owing to the structure $\lambda\, r(\lambda/k^2)$ of the regulator, one can apply a reparametrization $p^2 = \lambda^{-1}k^2$ which yields

$$\mathrm{Tr}_4\left\{\alpha\,\zeta_0^{-1}\Gamma_*\lim_{\lambda\to 0}\int_0^{k_0^2/\lambda} dp^2\;\theta(p^2\lambda)\left(-\frac{d}{dp^2}[R_p(1)+1]^{-1}-\frac{1}{2p^2}\eta_{\zeta_0}\frac{R_p(1)}{(R_p(1)+1)^2}\right)\right\}$$

Now the limit $\lambda\to 0$ can be performed. Note that a possible contribution from $p^2 = k_0^2/\lambda\to\infty$ is suppressed by the regulator expressions. The result is

$$\begin{aligned}&(\theta_{k_0^2}-\theta_0)\int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b \\ &=-\mathrm{Tr}_4\left\{\alpha\,\zeta_0^{-1}\Gamma_*\int_0^\infty dp^2\;\theta_0\left(\frac{d}{dp^2}[R_p(1)+1]^{-1}+\frac{1}{2p^2}\,\eta_{\zeta_0}\,\frac{R_p(1)}{(R_p(1)+1)^2}\right)\right\}\end{aligned} \tag{5.38}$$

The first part of the p-integral simply yields $-\theta_0$ due to $\lim_{p\to\infty}R_p(1)=\infty$ and $\lim_{p\to 0}R_p(1)=0$. In order to compute the second part one has to specify R_k. Using the optimized regulator, whose rescaled version reads $R_p(1)=(p^2-1)\Theta(p^2-1)$, the integral yields $\theta_0\,\frac{1}{35}\,\eta_{\zeta_0}$, such that

$$(\theta_{k_0^2}-\theta_0)\int d^2x\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\;\alpha\;\partial_\mu\varphi^a\partial_\nu\varphi^b=\frac{\theta_0}{\zeta_0}\left(1-\frac{1}{35}\eta_{\zeta_0}\right)\mathrm{Tr}_4\{\alpha\Gamma_*\}\,. \tag{5.39}$$

The trace $\mathrm{Tr}_4\,\{\alpha\Gamma_*\}$ ought to be considered in the regularized form $\lim_{s\to 0}\mathrm{Tr}_4\{\alpha\Gamma_*\mathrm{e}^{s\not{D}^2}\}$. It represents the analytical index of $-\not{D}^2$ and can be directly related to the topological index according to the Atiyah-Singer index theorem [125].

In order to compute $\lim_{s\to 0}\mathrm{Tr}_4\{\alpha\Gamma_*\mathrm{e}^{s\not{D}^2}\}$ one can employ a heat kernel expansion similiar to Eq. (5.13). Starting with the ansatz

$$\langle x|\mathrm{e}^{s\not{D}^2}|y\rangle=\frac{1}{4\pi s}\,\mathrm{e}^{-\frac{|x-y|^2}{4s}}\sum_{n=0}^\infty s^n C_n(x,y)\,, \tag{5.40}$$

where C_n are 4×4 matrices defined on the tensor product of the target space with itself, constraints for these coefficients can be derived in the same way as in Eq. (5.14) and read

$$n\,C_n+(x-y)^\mu\begin{bmatrix}\nabla_\mu & 0\\ 0 & \nabla_\mu\end{bmatrix}C_n-\begin{bmatrix}\nabla^\mu\nabla_\mu+\epsilon_{ab}\epsilon^{\mu\nu}\nabla_\mu\nabla_\nu & 0\\ 0 & \nabla^\mu\nabla_\mu-\epsilon_{ab}\epsilon^{\mu\nu}\nabla_\mu\nabla_\nu\end{bmatrix}C_{n-1}=0.$$

The relevant contribution to the index is provided by C_1, since all higher coefficients are suppressed in the limit $s\to 0$, while C_0 only yields a field-independent vacuum renormalization. The coefficient C_1 can be constructed from the solution

$$C_0 = \begin{bmatrix} c_0 & 0 \\ 0 & c_0 \end{bmatrix}\ , \text{ with } c_0 \text{ given in Eq. (5.15)}\,, \tag{5.41}$$

analogously to (5.18) as

$$C_1 = \begin{bmatrix} c_1^+ & 0 \\ 0 & c_1^- \end{bmatrix} \quad \text{with} \quad c_1^+ = c_0 \int_0^1 d\lambda\ \left(c_0^{-1}\left(\nabla^\mu\nabla_\mu + \epsilon_{ab}\epsilon^{\mu\nu}\nabla_\mu\nabla_\nu\right)c_0\right)^{*\lambda}$$
$$c_1^- = c_0 \int_0^1 d\lambda\ \left(c_0^{-1}\left(\nabla^\mu\nabla_\mu - \epsilon_{ab}\epsilon^{\mu\nu}\nabla_\mu\nabla_\nu\right)c_0\right)^{*\lambda}\,. \tag{5.42}$$

Multiplying C_1 by Γ_* and taking the trace, the terms containing $\nabla^\mu\nabla_\mu$ cancel each other, while the terms containing $\epsilon_{ab}\epsilon^{\mu\nu}\nabla_\mu\nabla_\nu$ add up. They can be written as

$$2\,\epsilon_{ac}\epsilon^{\mu\nu}\left(\nabla_\mu\nabla_\nu\right)^c{}_b = \epsilon_{ac}\epsilon^{\mu\nu}R^c{}_{bde}\partial_\mu\varphi^d\partial_\nu\varphi^e = 2\,\epsilon_{ad}\epsilon^{\mu\nu}\partial_\mu\varphi^d\partial_\nu\varphi_b\,. \tag{5.43}$$

Finally, the coincidence limit $y \to x$ is taken such that $c_0 \to \mathbb{1}_2$ and the trace yields

$$\lim_{s\to 0}\mathrm{Tr}_4\left\{\alpha\Gamma_*\mathrm{e}^{s\not{D}^2}\right\} = -\frac{1}{2\pi}\int d^2x\,\epsilon^{\mu\nu}\sqrt{h}\epsilon_{ab}\ \alpha\ \partial_\mu\varphi^a\partial_\nu\varphi^b\,. \tag{5.44}$$

Using this result in Eq. (5.39) one obtains an explicit expression for the renormalization of θ in the extreme IR:

$$\theta_{k_0^2} - \theta_0 = -\frac{1}{2\pi}\frac{\theta_0}{\zeta_0}\left(1 - \frac{1}{35}\eta_{\zeta_0}\right)\,. \tag{5.45}$$

Since the topological parameter θ_k does not run from the UV down to any finite scale k_0, the relation between bare and full effective coupling is solely determined by this "jump" in the IR and reads

$$\theta_0 = \left(1 - \tfrac{1}{2\pi}\left(1 - \tfrac{1}{35}\eta_{\zeta_0}\right)\zeta_0^{-1}\right)^{-1}\theta_\infty\,. \tag{5.46}$$

Inserting the result (5.10) for $\dot{\zeta}_0$ and rearranging the expression leads to

$$\theta_0 = \frac{2\pi\,\zeta_0\left(4\pi\,\zeta_0 - 1\right)}{8\pi^2\,\zeta_0^2 - 6\pi\,\zeta_0 + \frac{33}{35}}\ \theta_\infty\,. \tag{5.47}$$

The bare and the renormalized parameter are linearly related by a factor that depends only on the effective coupling ζ_0 in the infrared. The nonlinear O(3) model apparently constitutes another example of a theory with topological term in which the corresponding parameter is affected by a renormalization in the IR, similar to Yang-Mills and Chern-Simons theory [28, 29]. It should be emphasized, yet, that the derivation of (5.47) relied on a generalization of the topological operator by introducing an auxiliary field, for which the limit corresponding to the actual winding number is considered at the end. The physical interpretation of this construction amounts to a topological term which arises from an interaction with a scalar field that assumes a constant expectation value at the end.
The observed renormalization is an effect of the extreme IR. It thus seems to be impossible to investigate this issue further by means of methods like e.g. lattice computations, which are restricted to finite volumnes. On the other hand, result (5.47) does not contradict recent numerical simulations [117, 120] which showed that the θ-term is a relevant operator and does not renormalize to zero[8].
A comment on the periodicity properties shall conclude this discussion: The topological charge is introduced as a phase in the path integral and since the winding number Q assumes integer values for smooth fields, one would expect that the physical properties of the theory are 2π-periodic in θ. The renormalization derived in (5.47), however, is linear in θ. Although many other analytic and numerical computations, cf. for instance [115, 118, 59], also lack periodicity, it yet demands an explanation. It was conjectured in [59] that the $|\theta| > \pi$ vacua of the model suffer from a strongly increased pair production which leads to a break down of these vacua until values $|\theta| < \pi$ are reached. This conjecture was motivated by such findings in the massive Schwinger model [126, 127] which has similar properties as the CP^n models with regard to the vacua properties. In fact, recent large-n computations [128] indicate that such effects are present in CP^n models as well. Following this argumentation, one should trust the result (5.47) only for $\theta < \pi$.

5.5. Conclusions

The renormalization of the topological charge in the $CP^1 \cong \mathrm{O}(3)$ nonlinear sigma model was studied by means of the Functional Renormalization Group. A similar approach could be applied as in Yang-Mills theory [28] where a nontrivial renormalization of the topological operator was found in the extreme UV and IR, by considering the topological term as a specific limit of a more general operator. In

[8]Note that the value of the pathologic $\zeta_0 = \frac{1}{4\pi}$ is only an artefact of the regulator choice.

order to compute the renormalization in the UV, an off-diagonal heat kernel expansion as well as a careful analysis of a coincidence limit were performed. The extreme IR was studied by means of a reformulation of the flow equation in terms of a specific representation of the Clifford algebra, which enabled to compute the contributions of zero modes using the index theorem.

The analysis showed that a possible renormalization of θ in the UV is suppressed by the asymptotic freedom of the model. In the IR, however, a discrete and finite renormalization occurs as an effect of zero modes. In accordance with the findings in Yang-Mills and Chern-Simons theories [28, 29], this article thus provides further evidence that topological operators can be affected by a renormalization in the extreme IR. It should be kept in mind, however, that the calculations rely on the interpretation of the topological charge as a certain limit of an interaction with an auxiliary field which finally assumes a constant value.

6. Supersymmetric Extentions and their Discretizations

The analysis presented in this chapter originates from a collaboration with Daniel Körner, Andreas Wipf and Christian Wozar and has already been presented in [129].

The idea of symmetry relations between bosonic and fermionic degrees of freedom, denoted as *supersymmetry*, first arose in dual models which were an early version of string theory [130, 131, 132], and independently in [133]. It quickly gained attentation and supersymmetric field theories were developed systematically [134, 135, 136], motivated by two remarkable features of this concept: First, supersymmetry is interesting from a conceptual point of view, because it was proven (based on a small set of physically reasonable assumptions) that fermionic symmetry generators allow for the only possible nontrivial extension of the Poincaré symmetry [137, 35]. This extension is given in terms of a graded Lie algebra. The anticommutator of the supercharges Q_α, as the generators of supersymmetry transformations, is for example given by:

$$\{Q^I_\alpha, \bar{Q}^J_\beta\} = 2\mathrm{i}\,\delta^{IJ}\gamma^\mu_{\alpha\beta}\partial_\mu = 2\,\delta^{IJ}\gamma^\mu_{\alpha\beta}P_\mu\,, \quad I, J = 1, ..., \mathcal{N} \tag{6.1}$$

A characterstic property of theories with (unbroken) supersymmetry is the degeneracy of the energy spectrum, which is represented in the algebra by the commutator

$$\left[Q^I_\alpha, P_\mu\right] = 0\,, \qquad I = 1, ..., \mathcal{N}\,. \tag{6.2}$$

Each excited state is part of a multiplet of *superpartners* which have the same mass and are related by supersymmetry transformations.
The second motivation for the study of supersymmetry lies in model building and the attempt to solve open problems in particle physics. Owing to a cancellation of the quantum corrections coming from bosonic and fermionic superpartners, supersymmetric theories have improved renormalization properties. Particular interestingly aspects are the possibility to solve the hierarchy problem of the Higgs sector and to

unify electroweak and strong interactions at a high energy scale [138]. Besides this, supersymmetry has gained attention, as it naturally provides candidates for dark matter particles [139], and because analytical insights into a confinement mechanism have been obtained in supersymmetric extensions of gauge theory [140, 141]. Finally, supersymmetry is also an important building block of string theories.
Despite this theoretical motivation, there have been no experimental indications so far that supersymmetry is indeed realized in nature. The masses of the observed fermionic and bosonic particles are not degenerate, such that a mechanism would be required to explain the breaking of a possible fundamental supersymmetry. For this purpose many investigations of supersymmetry breaking have been performed and increasingly refined breaking mechanisms have been suggested, see e.g. [142, 143, 144, 145].
In spite of the strong interest in supersymmetric models, a non-pertubative investigation of these theories is restricted by a conceptual shortcoming of the lattice approach. Supersymmetry is an extension of spacetime symmetry and is hence broken by the discretization of a theory on the lattice. This breaking is inevitable, since the Leibniz rule cannot be implemented exactly on the lattice [146]. Even the restoration of supersymmetry in the continuum limit is not ensured, but requires the fine tuning of each relevant operators that is due to the symmetry breaking on the finite lattice. Since this procedure becomes unfeasible in most cases, alternative approaches have been developed with the aim to maintain at least a part of the supersymmetry on the lattice [147]. The expectation is that the full symmetry is automatically restored in the continuum limit without the need for fine tuning, if a part of the symmetry is already implemented on the lattice. One of these approaches relies on the possibility to combine supercharges in models with enlarged superalgebra, i.e. with $\mathcal{N} \geq 2$, such that they form a nilpotent operator $\mathcal{Q}$ which is employed to construct a $\mathcal{Q}$-exact formulation $S = \mathcal{Q}\Lambda$ of the lattice action, where Λ is some specific functional.
Since two-dimensional CP^n models are Kähler manifolds, it is possible to construct $\mathcal{N} = 2$ supersymmetric extensions of them [61] which can be used as testing ground for this procedure. These models provide a particular useful testing ground, since their numerical simulations require less computer resources than e.g. Yang-Mills theories. Furthermore, it was shown in [148] that the supersymmetry of these theories is not spontaneously broken, so that one can focus on the problem of the explicit breaking due to the discretization prescription. The $\mathcal{Q}$-exact approach outlined above was applied to the supersymmetric $\mathrm{CP}^1 \cong \mathrm{O}(3)$ model in [149, 150] and the investigations of Ward identities indicated the restoration of the full supersym-

metry in the continuum limit. However, the lattice discretization employed in these investigations explicitly breaks the O(3) symmetry of the theory and numerical simulations based on this lattice action reveal that the O(3) symmetry is not restored in the continuum limit. This lattice construction can thus not be identified with the two-dimensional nonlinear O(3) model[1]. The test simulations and measurements which show this failure are presented in more detail in [129].
A more precise analysis of the supersymmetric O(3) $\cong$ CP^1 model with particular emphasis on the interplay of O(3) and supersymmetry is hence required and shall be given in this chapter. Although it is crucial that the theory belongs to the class of CP^n models and hence exhibits an $\mathcal{N} = 2$ supersymmetry, the analysis will be developed in the formulation of the O(N) models, since the features of the O(3) symmetry are more transparent there. First, a brief introduction to the theory is given, before a supersymmetric version of the stereographic projection is developed. This projection will become useful in the construction of a lattice action and in the derivation of an expression for the second supersymmetry transformation in terms of explicitly constrained field variables. Based on the latter, the possibility to construct a $\mathcal{Q}$-exact lattice formulation can be analyzed. Finally, a supersymmetric Ward identity is briefly discussed, before a manifestly O(3) symmetric lattice action is presented for which explicit numerical results have been obtained.

6.1. Supersymmetric O(N) Models

Supersymmetric O(N) models were first discussed in [152] and [153]. A convenient way to derive the supersymmetric extension of nonlinear sigma models is provided by the superspace formalism [154]. Superspace is the extension of the usual spacetime by additional Grassmanian coordinates θ. Superfields are fields which are defined on this space (x, θ) and consists of bosonic and fermionic components. The supersymmetric extension of two-dimensional nonlinear O(N) models can be constructed in terms of constrained superfields $\boldsymbol{\Phi}$ which are real, bosonic N-tupels. They are defined on a superspace which consists of two real Grassmannian coordinates (θ_1, θ_2) that can be combined to a spinor θ. Owing to the nilpotency of these coordinates, the superfield can be expanded as

$$\boldsymbol{\Phi}(x, \theta) = \boldsymbol{n}(x) + \mathrm{i}\bar{\theta}\boldsymbol{\psi}(x) + \frac{\mathrm{i}}{2}\bar{\theta}\theta\boldsymbol{f}(x). \tag{6.3}$$

[1]Note that the O(3) symmetry of the model cannot be spontaneously broken due to the Mermin-Wagner theorem [151].

In accordance with the superfields also the components $\boldsymbol{n}$ and $\boldsymbol{f}$ are real, bosonic N-tupels, while $\boldsymbol{\psi}^\alpha$ ($\alpha = 1, 2$) denotes a fermionic N-tupel which fulfills the Majorana condition. The conventions concerning gamma matrices and the resulting Fierz relations are described in appendix A.2.
The constraint $\boldsymbol{n}^2 = 1$ of the bosonic fields can be promoted to the superfields, such that $\boldsymbol{\Phi}^2 = 1$. In terms of the component fields, this constraint amounts to

$$\boldsymbol{n}^2 = 1, \quad \boldsymbol{n}\cdot\boldsymbol{\psi}^\alpha = 0 \quad \text{and} \quad \boldsymbol{n}\cdot\boldsymbol{f} = \tfrac{\mathrm{i}}{2}\bar{\boldsymbol{\psi}}\boldsymbol{\psi}\,. \tag{6.4}$$

The generators Q_α of the first supersymmetry act on the space of superfields as

$$Q_\alpha = \frac{\partial}{\partial\bar\theta^\alpha} - \mathrm{i}\,(\gamma^\mu\theta)\partial_\mu, \qquad \bar{Q}_\alpha = -\frac{\partial}{\partial\theta^\alpha} + \mathrm{i}\,(\bar\theta\gamma^\mu)\partial_\mu\,, \tag{6.5}$$

and infinitesimal transformations are generated by $\bar\epsilon Q$ as

$$\delta_\epsilon\boldsymbol{n} = \mathrm{i}\bar\epsilon\boldsymbol{\psi}, \quad \delta_\epsilon\boldsymbol{\psi} = \not{\partial}\boldsymbol{n}\epsilon + \boldsymbol{f}\epsilon, \quad \delta_\epsilon\boldsymbol{f} = \mathrm{i}\bar\epsilon\not{\partial}\boldsymbol{\psi}\,. \tag{6.6}$$

The corresponding super-covariant derivative reads

$$D_\alpha = \frac{\partial}{\partial\bar\theta^\alpha} + \mathrm{i}\,(\gamma^\mu\theta)\partial_\mu, \qquad \bar{D}_\alpha = -\frac{\partial}{\partial\theta^\alpha} - \mathrm{i}\,(\bar\theta\gamma^\mu)\partial_\mu\,, \tag{6.7}$$

and anticommutes with the symmetry transformations. It is now simple to construct supersymmetric functionals as spacetime integrals of the coefficient[2] of $\bar\theta\theta$ in any covariant combination of fields $\boldsymbol{\Phi}$ and derivatives $D\boldsymbol{\Phi}$. This follows directly from (6.5), as supersymmetric transformations affect the term proportional to $\bar\theta\theta$ only by a total spacetime derivative. Due to the Grassmannian nature of these coordinates, the projection on the $\bar\theta\theta$-coefficient can be obtained by integration w.r.t. θ and $\bar\theta$. The supersymmetric extension of the O(N) models can hence be constructed as

$$S = \frac{1}{2g^2}\int d^2x d^2\theta\,\bar{D}\boldsymbol{\Phi}\,D\boldsymbol{\Phi} = \frac{1}{2g^2}\int d^2x\;\partial_\mu\boldsymbol{n}\partial^\mu\boldsymbol{n} + \mathrm{i}\bar{\boldsymbol{\psi}}\not{\partial}\boldsymbol{\psi} - \boldsymbol{f}^2\,. \tag{6.8}$$

By construction, the theory is invariant under the supersymmetry transformations (6.6) as well as O(N) transformations of $\boldsymbol{\Phi}$ or simultanously of $\boldsymbol{n}, \boldsymbol{\psi}$ and $\boldsymbol{f}$. Additionally, it exhibits a chiral $\mathbb{Z}_2$ symmetry $\boldsymbol{\psi} \to \mathrm{i}\gamma_*\boldsymbol{\psi}$ on the classical level. Quantum fluctuactions, however, dynamically generate a mass term and induce a spontaneous breaking of the chiral symmetry [155]. This mass gap could be determined in [156, 157] by comparing computations of the free energy obtained by the thermo-

[2] usually called D-term

dynamic Bethe ansatz and by perturbation theory. The former computations rely on the S-matrix of the theory which was derived in [158]. Since the bosonic field $\boldsymbol{f}$ appears only quadratic, it can be eliminated by a Gaussian integration. However, the constraint (6.4) has to be taken into account, such that the integration effects a substitution $\boldsymbol{f} = \frac{\mathrm{i}}{2}(\bar{\boldsymbol{\psi}}\boldsymbol{\psi})\boldsymbol{n}$. The on-shell action is thus

$$S[\boldsymbol{n}, \boldsymbol{\psi}] = \frac{1}{2g^2}\int d^2x\ \partial_\mu \boldsymbol{n}\partial^\mu \boldsymbol{n} + \mathrm{i}\bar{\boldsymbol{\psi}}\not{\partial}\boldsymbol{\psi} + \tfrac{1}{4}(\bar{\boldsymbol{\psi}}\boldsymbol{\psi})^2\,, \tag{6.9}$$

which is invariant under the on-shell supersymmetry transformations

$$\delta_\epsilon \boldsymbol{n} = \mathrm{i}\bar{\epsilon}\boldsymbol{\psi}, \quad \delta_\epsilon \boldsymbol{\psi}^\alpha = (\not{\partial}\boldsymbol{n}\epsilon)^\alpha + \tfrac{\mathrm{i}}{2}(\bar{\boldsymbol{\psi}}\boldsymbol{\psi})\,\boldsymbol{n}\,\epsilon^\alpha\,. \tag{6.10}$$

6.2. Supersymmetric Stereographic Projection

So far the explicitly constrained formulation of the theory has been considered. In order to analyze the model efficiently by means of numerical simulations, however, it is favorable to work with unconstrained dynamical degrees of freedom. Stereographic coordinates are a natural choice for this purpose and the stereographic projection (2.11) of bosonic fields can directly be extended to the superfields. A real, bosonic, but unconstrained superfield $\boldsymbol{U}(x,\theta) = \boldsymbol{u}(x) + \mathrm{i}\bar{\theta}\boldsymbol{\lambda}(x) + \frac{\mathrm{i}}{2}\bar{\theta}\theta\boldsymbol{g}(x)$ is introduced, which is related to $\boldsymbol{\Phi}$ by

$$\begin{pmatrix}\boldsymbol{\Phi}_\perp \\ \Phi_N\end{pmatrix} = \frac{1}{1+\boldsymbol{U}^2}\begin{pmatrix}2\boldsymbol{U} \\ 1-\boldsymbol{U}^2\end{pmatrix}\,, \qquad \text{with } \boldsymbol{\Phi}_\perp = (\Phi_1, ..., \Phi_{N\text{-}1})^\mathsf{T} \tag{6.11}$$

The superfield $\boldsymbol{U}$ as well as the bosonic fields $\boldsymbol{u}$ and $\boldsymbol{g}$ and the Majorana fermions $\boldsymbol{\lambda}^\alpha$ are $(N-1)$-tupels. The decomposition of this projection into field components reads:

$$\begin{aligned}
\begin{pmatrix}\boldsymbol{n}_\perp \\ n_N\end{pmatrix} &= \rho\begin{pmatrix}2\boldsymbol{u} \\ 1-\boldsymbol{u}^2\end{pmatrix}, \qquad\qquad \text{with } \rho = \frac{1}{1+\boldsymbol{u}^2} \\
\begin{pmatrix}\boldsymbol{\psi}_\perp^\alpha \\ \psi_N^\alpha\end{pmatrix} &= \rho\begin{pmatrix}2\boldsymbol{\lambda}^\alpha - 4\rho(\boldsymbol{u}\boldsymbol{\lambda}^\alpha)\boldsymbol{u} \\ -4\rho\boldsymbol{u}\boldsymbol{\lambda}^\alpha\end{pmatrix}, \\
\begin{pmatrix}\boldsymbol{f}_\perp \\ f_N\end{pmatrix} &= \rho\begin{pmatrix}2\boldsymbol{g} - 2\rho\,\boldsymbol{u}\big[2\boldsymbol{u}\boldsymbol{g} - \mathrm{i}\bar{\boldsymbol{\lambda}}\boldsymbol{\lambda} + 4\mathrm{i}\rho(\boldsymbol{u}\bar{\boldsymbol{\lambda}})(\boldsymbol{u}\boldsymbol{\lambda})\big] + 4\mathrm{i}\rho\bar{\boldsymbol{\lambda}}(\boldsymbol{u}\boldsymbol{\lambda}) \\ -4\rho\,\boldsymbol{u}\boldsymbol{g} + 2\mathrm{i}\rho(\bar{\boldsymbol{\lambda}}\boldsymbol{\lambda}) - 8\mathrm{i}\rho^2(\boldsymbol{u}\bar{\boldsymbol{\lambda}})(\boldsymbol{u}\boldsymbol{\lambda})\end{pmatrix}.
\end{aligned} \tag{6.12}$$

The inverse transformation in superspace is $\boldsymbol{U} = \boldsymbol{\Phi}_\perp/(1+\Phi_N)$ and it reads in terms of field components:

$$\begin{aligned} \boldsymbol{u} &= \frac{1}{2\rho}\,\boldsymbol{n}_\perp, \qquad\qquad \text{with } \rho = \frac{1+n_N}{2} \\ \boldsymbol{\lambda}^\alpha &= \frac{1}{2\rho}\,\boldsymbol{\psi}_\perp^\alpha - \frac{1}{4\rho^2}\,\psi_N^\alpha\,\boldsymbol{n}_\perp, \\ \boldsymbol{g} &= \frac{1}{2\rho}\,\boldsymbol{f}_\perp - \frac{1}{4\rho^2}\,f_N\,\boldsymbol{n}_\perp - \frac{\mathrm{i}}{4\rho^3}\,\bar{\psi}_N\psi_N\,\boldsymbol{n}_\perp + \frac{\mathrm{i}}{4\rho^2}\,\bar{\boldsymbol{\psi}}_\perp\psi_N. \end{aligned} \tag{6.13}$$

The constrained supersymmetric action is already given in its on-shell formulation (6.9), such that the projection relations of the auxiliary fields $\boldsymbol{f}$ and $\boldsymbol{g}$ are not relevant in the following analysis. Applying (6.12), an unconstrained formulation of the supersymmetric nonlinear O(N) model can be deduced from (6.9) as:

$$S[\boldsymbol{u},\boldsymbol{\lambda}] = \frac{2}{g^2}\int d^dx\;\rho^2\big(\partial_\mu\boldsymbol{u}\partial^\mu\boldsymbol{u} + \mathrm{i}\bar{\boldsymbol{\lambda}}\partial\!\!\!/\boldsymbol{\lambda} + 4\mathrm{i}\rho\,(\bar{\boldsymbol{\lambda}}\boldsymbol{u})\gamma^\mu(\boldsymbol{\lambda}\partial_\mu\boldsymbol{u}) + \rho^2(\bar{\boldsymbol{\lambda}}\boldsymbol{\lambda})^2\big)\,. \tag{6.14}$$

The corresponding supersymmetry transformations read:

$$\delta_\epsilon\boldsymbol{u} = \mathrm{i}\bar{\epsilon}\boldsymbol{\lambda}, \quad \delta_\epsilon\boldsymbol{\lambda}^\alpha = (\partial\!\!\!/\boldsymbol{u}\epsilon)^\alpha + \mathrm{i}\rho(\bar{\boldsymbol{\lambda}}\boldsymbol{\lambda})\boldsymbol{u}\,\epsilon^\alpha - 2\mathrm{i}\rho\,(\bar{\boldsymbol{\lambda}}\boldsymbol{u})\boldsymbol{\lambda}\,\epsilon^\alpha\,. \tag{6.15}$$

The coordinate transformation affects not only the action, but also the path integral measure. Since the measure is relevant in Monte Carlo simulations, the Jacobian of the stereographic projection should be studied in more detail, using a lattice regularization. Since the transformation only relates values of the fields on a fixed lattice site, it is sufficient to calculate the Jacobian for a given site. The only nontrivial factors in the measure of the constrained formulation are δ-functions which represent the constraints (6.4) for the fields $\boldsymbol{n}$ and $\boldsymbol{\psi}$. The stereographic projection is a transformation between $N-1$ degrees of freedom and the δ-functions ought to be considered as[3]

$$\begin{aligned} \delta(\boldsymbol{n}^2-1)\,\delta(\boldsymbol{n}\boldsymbol{\psi}^1)\,\delta(\boldsymbol{n}\boldsymbol{\psi}^2) &= \frac{1}{2|n_N|}\left[\delta\Big(n_N - \sqrt{1-\boldsymbol{n}_\perp^2}\,\Big) + \delta\Big(n_N + \sqrt{1-\boldsymbol{n}_\perp^2}\,\Big)\right]\times \\ &\quad\times\prod_{\alpha=1,2} n_N\,\delta\left(\psi_N^\alpha + \frac{\boldsymbol{n}_\perp\,\boldsymbol{\psi}_\perp^\alpha}{n_N}\right)\,. \end{aligned} \tag{6.16}$$

Consequently, the measure on a given site (whose index will be suppressed for simplicity) transforms as

$$\mathrm{d}\boldsymbol{n}\,\mathrm{d}\boldsymbol{\psi}^1\,\mathrm{d}\boldsymbol{\psi}^2\;\delta(\boldsymbol{n}^2-1)\delta(\boldsymbol{n}\cdot\boldsymbol{\psi}^1)\delta(\boldsymbol{n}\cdot\boldsymbol{\psi}^2) = \tfrac{1}{2}\;\mathrm{J}(\boldsymbol{u})\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{\lambda}^1\,\mathrm{d}\boldsymbol{\lambda}^2\,, \tag{6.17}$$

[3]Note that δ-functions of Grassmannian variables factorize linearly.

with the Jacobian

$$\mathrm{J}(\boldsymbol{u}) = \sqrt{1-\boldsymbol{n}_\perp^2(\boldsymbol{u})}\,\left|\mathrm{sdet}\{(\boldsymbol{n}_\perp,\boldsymbol{\psi}_\perp)\to(\boldsymbol{u},\boldsymbol{\lambda})\}\right| . \tag{6.18}$$

According to (6.12) $\boldsymbol{n}$ does not depend on $\boldsymbol{\lambda}^\alpha$, and $\boldsymbol{\psi}^\alpha$ does not depend on $\boldsymbol{\lambda}^\beta$ for $\beta \neq \alpha$. The superdeterminant is hence given by

$$\mathrm{sdet}\{(\boldsymbol{n}_\perp,\boldsymbol{\psi}_\perp)\to(\boldsymbol{u},\boldsymbol{\lambda})\} = \frac{\det(\partial\boldsymbol{n}_\perp/\partial\boldsymbol{u})}{\det(\partial\boldsymbol{\psi}_\perp^1/\partial\boldsymbol{\lambda}^1)\cdot\det(\partial\boldsymbol{\psi}_\perp^2/\partial\boldsymbol{\lambda}^2)} . \tag{6.19}$$

All three determinants are equal to

$$(2\rho)^{N-1}\,\frac{1-\boldsymbol{u}^2}{1+\boldsymbol{u}^2} \quad \text{with} \quad \rho = \frac{1}{1+\boldsymbol{u}^2} .$$

Expressing the square root in (6.18) in terms of the new fields,

$$\sqrt{1-\boldsymbol{n}_\perp} = \frac{1-\boldsymbol{u}^2}{1+\boldsymbol{u}^2},$$

the Jacobian finally reads

$$\mathrm{J}(\boldsymbol{u}) = \frac{1}{(2\rho)^{N-1}} \propto \left(1+\boldsymbol{u}^2\right)^{N-1} . \tag{6.20}$$

The functional integral measure for the supersymmetric O(3) model in stereographic coordinates is thus

$$\prod_x \mathrm{d}\boldsymbol{u}_x\,\mathrm{d}\boldsymbol{\lambda}_x^1\,\mathrm{d}\boldsymbol{\lambda}_x^2\,\left(1+\boldsymbol{u}_x^2\right)^2 . \tag{6.21}$$

Note that this computation verified that the Jacobian of the purely bosonic model is proportional to $\sqrt{h}$ with the metric $h_{ab} = \rho^2\delta_{ab}$:

$$\mathrm{J_B}(\boldsymbol{u}) \propto \rho^{N-1} = \frac{1}{(1+\boldsymbol{u}^2)^{N-1}} . \tag{6.22}$$

Note that in an off-shell formulation of the theory the superdeterminant of the transformation is multiplied by $\det(\partial\boldsymbol{f}_\perp/\partial\boldsymbol{g})$ and becomes the identity, as also $\det(\partial\boldsymbol{f}_\perp/\partial\boldsymbol{g}) = (2\rho)^{N-1}\,\frac{1-\boldsymbol{u}^2}{1+\boldsymbol{u}^2}$. Furthermore, there is an additional factor $|n_N|^{-1}$ due to the δ-function of the $\boldsymbol{f}$-constraint (6.4), such that the measure of the path integral in terms of stereographic coordinates is flat in the off-shell formulation[4]. This simplification provides a further example of a cancellation of fermionic and bosonic contributions due to superymmetry.

[4]If one integrates out the unconstrained auxiliary field $\boldsymbol{g}$ of the stereographic coordinates, one obviously reobtains the measure (6.20) coming from the coefficients of $\boldsymbol{g}$ in the action.

6.3. $\mathcal{N}=2$ Supersymmetry and Symmetric Discretizations

It was already mentioned in Sec. 2.3 that the target manifold of the bosonic $\mathrm{CP}^1 \cong \mathrm{O}(3)$ model is Kähler and the corresponding potential can be written in terms of the complex field $u = u_1 + iu_2$ as $K(u,\bar{u}) = \log(1+\bar{u}u)$. It was pointed out in [61] that a nonlinear sigma model whose target manifold is Kähler possesses an $\mathcal{N}=2$-supersymmetric extension. In order to determine the second supersymmetry of the O(3) model, one can study a generic ansatz in terms of the unconstrained fields ($\delta\boldsymbol{u} = \mathrm{i}\bar{\epsilon}(A_I)\boldsymbol{\lambda}$, etc.) and derive constraints for the matrices A_I, etc., from the supersymmetry algebra and the invariance of the action[5]. Following this approach, the second pair of supersymmetry transformations can be identified as

$$\delta\boldsymbol{u} = \sigma_2\bar{\epsilon}\boldsymbol{\lambda}\,,\quad \delta\boldsymbol{\lambda} = \mathrm{i}\sigma_2\left(\partial\!\!\!/\boldsymbol{u} - \mathrm{i}\rho\,(\bar{\boldsymbol{\lambda}}\boldsymbol{\lambda})\boldsymbol{u} + 2\mathrm{i}\rho\,(\bar{\boldsymbol{\lambda}}\boldsymbol{u})\boldsymbol{\lambda}\right)\epsilon\,, \tag{6.23}$$

where σ_2 denotes the second Pauli matrix, which does not act on spinor indices here, but on the field components. Both supersymmetries (6.15,6.23) can also be obtained by deriving the complex supersymmetry from the Kähler potential, cf. [61], and decomposing the complex fields and complex transformation parameters into real ones.
It is interesting to see how the second supersymmetry, which is only present in the case $N=3$ but not in generic $\mathrm{O}(N)$ models, reads in terms of constrained field variables. In order to derive this expression the inverse stereographic projection (6.13) can be applied to (6.23) and one obtains the concise expression

$$\begin{aligned} \delta\boldsymbol{n} &= \ \mathrm{i}\boldsymbol{n}\times\bar{\epsilon}\boldsymbol{\psi}\,, \\ \delta\boldsymbol{\psi} &= -\boldsymbol{n}\times\partial_\mu\boldsymbol{n}\,\gamma^\mu\epsilon - \mathrm{i}\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi}\,, \end{aligned} \tag{6.24}$$

where $\times$ denotes the vector product of three-tupels. The nontrivial proof that the action (6.9) is invariant under these transformations is presented in appendix A.3. The on-shell supersymmetries (6.10) and (6.24) are generated by the supercharges

$$Q^{\mathrm{I}} = \mathrm{i}\int\gamma^\mu\gamma^0\boldsymbol{\psi}\partial_\mu\boldsymbol{n}\,,\quad Q^{\mathrm{II}} = -\mathrm{i}\int\gamma^\mu\gamma^0\boldsymbol{\psi}(\boldsymbol{n}\times\partial_\mu\boldsymbol{n})\,. \tag{6.25}$$

This result is in agreement with the supercurrents constructed in [152].

[5] A more detailed example of this approach can be found in [159], where it is applied to the Wess-Zumino model.

As mentioned in the introduction of this chapter, it is possible in some theories with $\mathcal{N} \geq 2$ superalgebra to formulate a lattice action which is invariant under a part of the supersymmetry by constructing a nilpotent supercharge $\mathcal{Q}$ such that the lattice action can be written as $S = \mathcal{Q}\Lambda$. This approach is applied to the nonlinear O(3) model in [149, 150], but the chosen lattice discretization breaks the O(3) symmetry and cannot restore it in the continuum limit. This raises the question if there are other ways to find a partly supersymmetric but still O(3) symmetric discretization?

A symmetry of the model has to be a symmetry of the action (6.9), but is also has to be compatible with the constraints $\boldsymbol{n}^2 = 1$ and $\boldsymbol{n}\boldsymbol{\psi} = 0$. Any supersymmetry has to be a combination of the transformations given in (6.10) and (6.24). If one considers the discretization of these, one notices that the first transformation (6.10) breaks the constraint $\boldsymbol{n}\boldsymbol{\psi} = 0$ on the lattice[6], because

$$\delta_{\mathrm{I}}(\boldsymbol{n}_x\boldsymbol{\psi}_x^\alpha) = \mathrm{i}\bar{\epsilon}\boldsymbol{\psi}_x\boldsymbol{\psi}_x^\alpha + \sum_{y\in G}\boldsymbol{n}_x D_{xy}^{\alpha\beta}\boldsymbol{n}_y\epsilon^\beta + \tfrac{\mathrm{i}}{2}(\bar{\boldsymbol{\psi}}_x\boldsymbol{\psi}_x)\boldsymbol{n}_x^2\epsilon^\alpha \overset{(A.9)}{=} \sum_{y\in G}\boldsymbol{n}_x D_{xy}^{\alpha\beta}\boldsymbol{n}_y\epsilon^\beta, \quad (6.26)$$

where the subscripts x, y denote lattice sites and G the set of all these sites. The variation of the constraint does not vanish for arbitrary $\boldsymbol{n}_x$, no matter which lattice derivative D_{xy} one uses, since the Leibniz rule is broken on the lattice [146]. In contrast, the second transformation respects the constraints at each lattice site[7]:

$$\begin{aligned} \delta_{\mathrm{II}}(\boldsymbol{n}_x\boldsymbol{\psi}_x) &= \mathrm{i}(\boldsymbol{n}_x \times \bar{\epsilon}\boldsymbol{\psi}_x)\cdot\boldsymbol{\psi}_x - \sum_{y\in G}\boldsymbol{n}_x\cdot(\boldsymbol{n}_x \times D_{xy}\boldsymbol{n}_y\epsilon) - \mathrm{i}\boldsymbol{n}_x\cdot(\bar{\epsilon}\boldsymbol{\psi}_x \times \boldsymbol{\psi}_x) = 0 \\ \delta_{\mathrm{II}}(\boldsymbol{n}_x^2) &= 2\mathrm{i}\boldsymbol{n}_x\cdot(\boldsymbol{n}_x \times \bar{\epsilon}\boldsymbol{\psi}_x) = 0\,. \end{aligned} \quad (6.27)$$

One can conclude that no nontrivial combination of the two transformations δ_{I} and δ_{II} can be a symmetry of the lattice theory, since the second transformation cannot restore the violation of the constraints caused by the first one. The second transformation on its own, however, cannot be a symmetry of the action because of $\{Q_\alpha^{\mathrm{II}}, \bar{Q}_\beta^{\mathrm{II}}\} = 2i\gamma^\mu_{\alpha\beta}\partial_\mu$. The superalgebra furthermore shows that an approach based on a nilpotent supercharge is not possible, either, because a nilpotent charge has to be a combination of both charges Q^{I} and Q^{II} and hence violates the constraints.

Could one circumvent this restriction by "improving" the lattice action? Comparing the formulation used in this chapter with the one investigated in [149, 150], one sees that the latter one contains an additional topological term. However,

[6]Actually, it is also not a symmetry of the discretized action, but the breaking of the constraints is more severe.

[7]taking into account the cyclicality of the triple product

such a term does not affect the supersymmetry transformations (6.10) and (6.24) and hence cannot solve the problem. From a systematic point of view, there are only two modifications possible which are compatible with an O(3)-invariant continuum limit. The first possibility is to modify the terms that are already present in the action. For example, one could introduce non-local interaction terms like $\sum_{x,y,z,w} C_{xyzw}(\bar{\boldsymbol{\psi}}_x\boldsymbol{\psi}_y)(\bar{\boldsymbol{\psi}}_z\boldsymbol{\psi}_w)$ instead of $\sum_x(\bar{\boldsymbol{\psi}}_x\boldsymbol{\psi}_x)^2$ [160]. The second possibility could be an inclusion of additional terms in the lattice action which vanish in the continuum limit. Any change of the action, however, does not have an impact on the constraints and hence cannot prevent their breaking. A modification of the constraints, by contrast, would directly alter the geometry of the target manifold and is thus no alternative. It follows that an improvement of the discretization could only maintain a part of supersymmetry by rendering the lattice action invariant under the second transformations. But this is not possible due to the structure of the superalgebra.

Although these arguments were developed for a specific choice of coordinates, they also hold true for any reparametrization $(\boldsymbol{n},\boldsymbol{\psi}) \to (\boldsymbol{n}',\boldsymbol{\psi}')$, because such a transformation is a bijective mapping between field values at a certain point x in space-time, which commutes with discretization. As a consequence, one will observe the same pattern of symmetry breaking as depicted in (6.26) and (6.27) in any other parametrization. The single ambiguity which could arise from the discretized derivative of the bosonic field is irrelevant since the presented arguments do not depend on the details of the lattice derivatives.

One has to conclude that it is simply not possible to construct a discretization of the nonlinear O(3) model which maintains O(3) invariance as well as an exact supersymmetry. From this point of view, the symmetry breaking that occurs in the ansatz of [149, 150] is inevitable.

Since this analysis is based on the specific geometrical features of the CP^1 model, one cannot immediately draw analogous conclusions for general supersymmetric CP^n models. This issue requires more consideration.

6.4. O(3) Symmetric Discretization and Simulations

Since both symmetries cannot be maintained simultanously and since the $\mathcal{Q}$-exact formulation is not able to provide an appropriate continuum limit, it is reasonable to study the system in an O(3) symmetric discretization which breaks the supersymmetries, but aims to restore these in the continuum limit. In order to obtain such a discretization, one ought to start with the manifestly O(3) symmetric formulation given in (6.9). The corresponding lattice action reads

$$S[\boldsymbol{n},\boldsymbol{\psi}] = \frac{1}{2g^2}\sum_{x,y\in G}\left(\boldsymbol{n}_x^{\mathsf{T}}K_{xy}\boldsymbol{n}_y + \mathrm{i}\bar{\boldsymbol{\psi}}_x^{\alpha}M_{xy}^{\alpha\beta}\boldsymbol{\psi}_y^{\beta} + \tfrac{1}{4}(\bar{\boldsymbol{\psi}}_x\delta_{xy}\boldsymbol{\psi}_y)^2\right), \tag{6.28}$$

where α, β denote spinor indices and K_{xy} and $M_{xy}^{\alpha\beta}$ represent lattice derivatives, which are proportional to the identity w.r.t. the O(3) indices. In a next step, the discretized action (6.28) can be stereographically projected, so that the Monte Carlo algorithm can be implemented in terms of unconstrained dynamical variables. If one directly discretized the unconstrained formulation (6.14), ambiguities would arise concerning the discretization of the metrical factors in front of the kinetic terms. For instance, it is not clear a priori if $\rho_x\rho_y$ or $\frac{1}{2}(\rho_x^2+\rho_y^2)$ is the correct discretization of ρ^2 in front of $\partial_\mu\boldsymbol{u}\partial^\mu\boldsymbol{u} \mathrel{\hat{=}} \boldsymbol{u}_x\sum_y\Delta_{xy}\boldsymbol{u}_y$ in order to maintain O(3) invariance[8]. The outlined procedure based on the stereographic projection, however, proves that the geometric mean $\rho_x\rho_y$ is in fact the right choice. Applying (6.12) to (6.28) yields the manifestly O(3) symmetric and unconstrained discretization

$$\begin{aligned}
S[\boldsymbol{u},\boldsymbol{\lambda}] &= S_{\mathrm{B}} + S_{2\mathrm{F}} + S_{4\mathrm{F}}\,,\ \text{ with}\\
S_{\mathrm{B}} &= \frac{1}{2g^2}\sum_{x,y}4\rho_x\boldsymbol{u}_x^{\mathsf{T}}K_{xy}\boldsymbol{u}_y\rho_y + \rho_x(1-\boldsymbol{u}_x^2)K_{xy}(1-\boldsymbol{u}_y^2)\rho_y\,,\\
S_{2\mathrm{F}} &= \frac{2\mathrm{i}}{g^2}\sum_{x,y;\alpha,\beta}\bar{\boldsymbol{\lambda}}_x^{\alpha}\Big[\left(\rho-2\rho^2\boldsymbol{u}\,\boldsymbol{u}^{\mathsf{T}}\right)_x M_{xy}^{\alpha\beta}\left(\rho-2\rho^2\boldsymbol{u}\,\boldsymbol{u}^{\mathsf{T}}\right)_y + 4\left(\rho^2\boldsymbol{u}\right)_x M_{xy}^{\alpha\beta}\left(\rho^2\boldsymbol{u}^{\mathsf{T}}\right)_y\Big]\boldsymbol{\lambda}_y^{\beta}\,,\\
S_{4\mathrm{F}} &= \frac{2}{g^2}\sum_x\rho_x^4(\bar{\boldsymbol{\lambda}}_x\boldsymbol{\lambda}_x)^2\,.
\end{aligned}\tag{6.29}$$

As described above, the reparametrization yields the nontrivial Jacobian:

$$\prod_{x\in G}\mathrm{d}\boldsymbol{n}_x\,\mathrm{d}\boldsymbol{\psi}_x^1\,\mathrm{d}\boldsymbol{\psi}_x^2\;\delta(\boldsymbol{n}_x^2-1)\delta(\boldsymbol{n}\boldsymbol{\psi}_x^1)\delta(\boldsymbol{n}\boldsymbol{\psi}_x^2)\longrightarrow\prod_{x\in G}\mathrm{d}\boldsymbol{u}_x\,\mathrm{d}\boldsymbol{\lambda}_x^1\,\mathrm{d}\boldsymbol{\lambda}_x^1\;\left(1+\boldsymbol{u}_x^2\right)^2\,.$$

The measure can be absorbed into the action as $S_m = -2\sum_x\log(1+\boldsymbol{u}_x^2)$. Moreover, the four-fermion interaction can be eliminated by a Hubbard-Stratonovich transformation [161], which introduces an auxiliary bosonic field σ:

$$S[\boldsymbol{u},\boldsymbol{\lambda}] = S_{\mathrm{B}} + S_{2\mathrm{F}} + \frac{1}{2g^2}\sum_{x\in G}\left(\sigma_x^2 + 4\mathrm{i}\sigma_x\rho_x^2\,\bar{\boldsymbol{\lambda}}_x\boldsymbol{\lambda}_x\right) \tag{6.30}$$

The action is then quadratic in the fermionic fields, i.e. $\tilde{S}_{\mathrm{F}} = \sum_{x\in G}\bar{\boldsymbol{\lambda}}_x\,Q_{xy}^{\mathrm{F}}(\boldsymbol{u},\sigma)\,\boldsymbol{\lambda}_y$, and a Gaussian integral can be performed formally. The fermion determinant, i.e.

[8] This is actually the critical point which leads to a symmetry breaking in [149, 150].

more precisely the Pfaffian[9] $\mathrm{Pf}\, Q^{\mathrm{F}} = (\det Q^{\mathrm{F}})^{1/2}$ which appears in the measure is a function of bosonic fields only and can be incorporated in the action as well. The result is a purely bosonic path integral which can be efficiently investigated by Monte Carlo methods:

$$\begin{aligned}\mathcal{Z} &= \int \prod_{x\in G} \mathrm{d}\boldsymbol{u}_x \mathrm{d}\sigma_x \; (\det Q^{\mathrm{F}})^{1/2}\; \mathrm{e}^{-\tilde{S}_{\mathrm{B}} - S_m}\,, \qquad \tilde{S}_{\mathrm{B}} = S_{\mathrm{B}} + \frac{1}{2g^2}\sum_{x\in G}\sigma_x^2\,, \\ &= \int \prod_{x\in G} \mathrm{d}\boldsymbol{u}_x \mathrm{d}\sigma_x \; \mathrm{e}^{-\tilde{S}_{\mathrm{B}}[\boldsymbol{u},\sigma] - S_m[\boldsymbol{u}] + \frac{1}{2}\log\det Q^{\mathrm{F}}[\boldsymbol{u},\sigma]}\,. \end{aligned} \tag{6.31}$$

Since the supersymmetry of the continuum $\mathrm{CP}^1 = O(3)$ model is neither spontaneously nor explicitly broken, the bosonic and fermionic masses in the numerical simulations ought to be degenerate in the continuum limit, where the explicit breaking induced by a finite lattice spacing vanishes. The masses hence serve as a direct indicator of supersymmetry restoration.

Besides the mass degeneracy, also the supersymmetric Ward identity derived for the bosonic action in [149, 150] is comparably easy to access and will serve as benchmark for the restoration of supersymmetry. The lattice action in [149, 150] can be written in terms of a nilpotent charge $\mathcal{Q}$ as $S = g^{-2}\mathcal{Q}\Lambda$ and it differs from the lattice action studied here only by surface terms which should become negligible on sufficiently large lattices. Since the action as well as the measure are invariant under the supercharge Q, the following relation holds true for the supersymmetric continuum theory:

$$\frac{\partial \ln \mathcal{Z}}{\partial(g^{-2})} = \langle -\mathcal{Q}\Lambda\rangle = 0\,. \tag{6.32}$$

Since the field-independent factors in the partition sum $\mathcal{Z}$ are usually not relevant, it was not made explicit in (6.31), but the path integral measure of $\mathcal{Z}$ actually contains the factor g^V, where V denotes the total number of lattice sites. The integration of the auxiliary field is a Gaußian integration of two independent degrees of freedom at each lattice site which provides a factor g^{2V}. This is partly compensated by the factor g^{-V} that accompanies the introduction of the field σ. The fermion operator Q^{F} is proportional to g^{-2}, so that its determinant is proportional to $g^{-2\cdot\dim Q^{\mathrm{F}}}$, where $\dim Q^{\mathrm{F}}$ is the dimension of the fermion operator in terms of O(3) and spinor components as well as lattices sites. The differentiation of (6.31) hence yields

$$\frac{\partial \ln \mathcal{Z}}{\partial(g^{-2})} = -\frac{1}{2}Vg^2 - g^2\left\langle \tilde{S}_{\mathrm{B}}\right\rangle + \frac{1}{2}\,g^2\dim Q^{\mathrm{F}}\,. \tag{6.33}$$

[9] For the sake of simplicity, the sign of the Pfaffian will be ignored in the discussion here.

In the investigated lattice system is $\dim Q^{\mathrm{F}} = 4V$ and the supersymmetric Ward identity (6.32) is hence fulfilled if

$$\left\langle \tilde{S}_{\mathrm{B}} \right\rangle = \frac{3}{2} V \,. \tag{6.34}$$

Having two indicators of supersymmetry restoration, one can now proceed to study explicit numerical computations. Since the implementation of the algorithm and the measurements on the resulting configurations were done by Daniel Körner, only the important results shall be briefly presented in this thesis, while a more detailed discussion can be found in [129].
Based on the lattice discretization described in this section, numerical simulations have been performed on $N_t \times N_s = 8 \times 8, 16 \times 16$ and 24×24 lattices by means of an HMC algorithm which employs *Wilson derivatives*:

$$M^{\alpha\beta}_{xy} = \gamma^{\alpha\beta}_{\mu} \left(\partial^{\mathrm{sym}}_{\mu}\right)_{xy} + \delta^{\alpha\beta} \frac{ra}{2} \Delta_{xy} \,, \quad K_{xy} = -\left(\partial^{\mathrm{sym}}_{\mu}\right)^2_{xy} + \left(\frac{ra}{2} \Delta_{xy}\right)^2 , \tag{6.35}$$

where $\partial^{\mathrm{sym}}_{\mu}$ is the symmetric lattice derivative, Δ_{xy} the lattice Laplacian, a the lattice spacing, and r some mass parameter that is introduces in order to suppress fermion doublers, see [14]. The Wilson derivatives provide an ultralocal implementation of the derivative operators, but have the disadvantage that the introduction of the mass term leads to an explicit breaking of the chiral symmetry[10]. Further details of the implementation as well as an alternative formulation based on group valued variables and the *SLAC derivative* are given in [129].
In case of intact O(3) symmetry, the expectation value of the constrained fields should vanish, e.g. $\langle \boldsymbol{n} \rangle = 0$. It was confirmed that this holds true and the Monte Carlo computations are in fact invariant under O(3) transformations[11]. In order to investigate supersymmetry, the masses are determined from the O(3) symmetric two-point functions, which can easily be measured on the configurations. The exponential decrease of the two-point functions in time direction depends on the energy of the states. The mass can be determined from a cosh-fit of the two-point functions[12], based on the assumption that the lowest eigenstate, i.e. the mass of the ground state, dominates the faster-decresasing excited states for sufficiently large lattices. The only quantities in the simulations that provide a unit of lenghts (or

[10]Note that is is not possible to construct a lattice formulation of fermions in terms of local interactions which maintains chiral symmetry exact (without introducing additional flavors) [162].

[11]There may occur a problematic interplay between the stereographic projection and the HMC momenta, but this can be resolved by a simple algorithmic modification.

[12]A cosh-fit has to be applied due to the finite, periodic length of the lattice.

inverse energy) are the lattice spacing a or the lattice length $L = aN_s$. Physically meaningful expressions of the masses have hence to be given in units of a^{-1} or L^{-1}. In case of supersymmetry the masses of bosonic and fermionic degrees of freedom ought to be degenerate. The left panel of Fig. 6.1 displays the relation between these masses for three different lattices sizes V and for different physical lengths L (which are implicitly measured in units of m_F)[13]. It shows that no mass degeneracy can be obtained, not even in the continuum limit (which means larger lattices at fixed physical volumne), but there is an increasing gap between bosonic and fermionic masses instead.

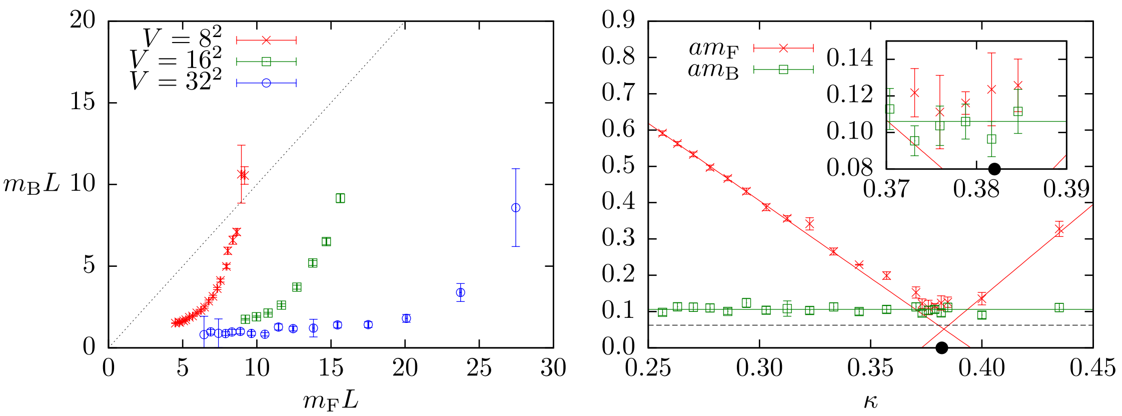

Figure 6.1.: Left Panel: Comparison of bosonic and fermionic masses in units of the box size L for three different lattice sizes V using Wilson fermions. The dotted line denotes the case $m_F = m_B$. Right Panel: Scaling behaviour of the bosonic and fermionic mass w.r.t. the fine tuning parameter κ for $N = 16^2$ and $g^{-2} = 1.4$. $\kappa_c = 0.382(1)$ is marked by the black dot. The dashed line denotes the lattice cutoff of $1/16$.

This lack of a supersymmetric continuum limit is in fact not really surprising, as the explicit breaking at finite lattice spacing, which is further amplified by the mass term of the Wilson derivative, generates relevant operators with respect to renormalization. In order to compensate for these, one has to introduce counter terms by means of a fine tuning procedure. Inspired by a similar issue in case of $\mathcal{N} = 1$ super Yang-Mills theory [163], a fine tuning mass parameter m has been included in the computations by a modification of the fermionic derivative operator

$$M_{xy}^{\alpha\beta} \to M_{xy}^{\alpha\beta} + m\,\delta^{\alpha\beta}\delta_{xy}.$$

Similar to the case in super Yang-Mills theory, a useful indicator for the right choice of m is given by the chiral condensate. For the critical value at which the explicit

[13]The physical length or the physical size of the spacing depend on the value set for g.

breaking of the chiral symmetry due to the Wilson mass is compensated, the condensate increases sharply and one obtains the signature of a discrete chiral symmetry which is only spontaneously broken (and additively renormalized); cf. [129] for more details.

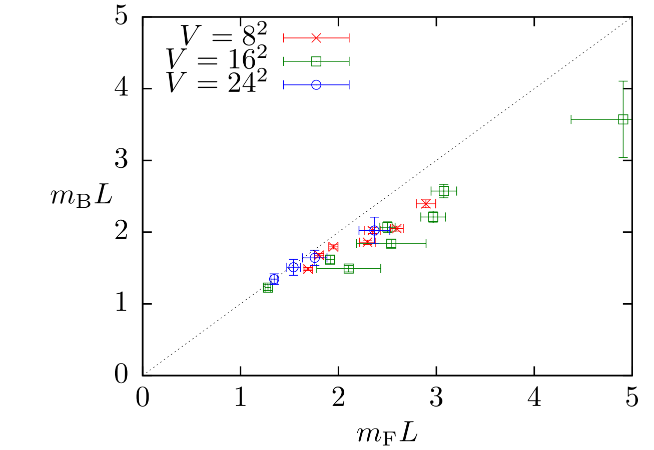

Figure 6.2.: Comparison of bosonic and fermionic masses in units of the box size L for three different lattice sizes at $\kappa = \kappa_c$.

The right panel of Fig. 6.1 shows how the fermionic mass decreases linearly with increasing fine tuning parameter $\kappa = (4 + 2m)^{-1}$, while the bosons are unaffected. For the critical fine tuning κ_c the masses are degenerate, whereas the discrepancy grows again if one increases κ further. As depicted in Fig. 6.2, measurements on different lattices confirm the degeneracy of fermionic and bosonic masses, if m is tuned to the value suggested by the chiral condensate. The results indicate that the degeneracy is stable for increasing lattices sizes and it hence seems possible to obtain a supersymmetric continuum limit by introducing only one fine tuning parameter.

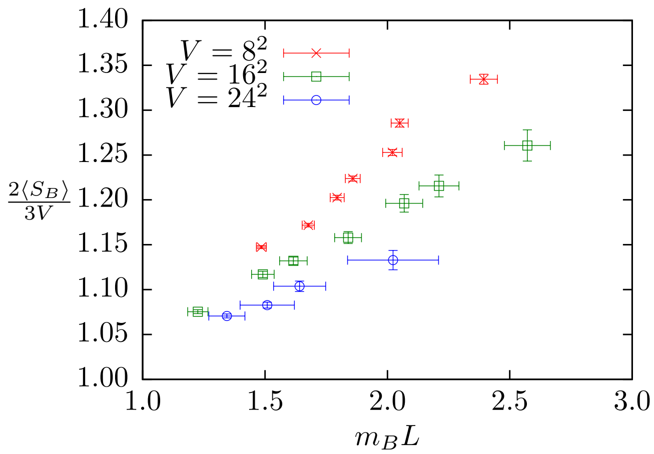

Figure 6.3.: Expectation value of the bosonic action $\tilde{S}_\mathrm{B}$ at $\kappa = \kappa_c$ for different box sizes L. In the supersymmetric continuum limit one expects $\frac{2\langle \tilde{S}_B \rangle}{3V} = 1$.

This agrees with the measurements of the Ward identity for the bosonic action. The expectation value of $\tilde{S}_{\mathrm{B}}$ is displayed in Fig. 6.3, calculated on different lattice sizes and different physical volumes. Although the deviation from the expected result $\frac{3}{2}V$ is more than 7%, the expectation value seems to approach the correct continuum limit for increasing lattice sizes.

6.5. Conclusions

In this chapter the supersymmetric extension of the nonlinear O(3) model was analyzed with particular interest in the discretization of supersymmetric theories. After an introduction to the concept of supersymmetry and to the specific model, a supersymmetric version of the stereographic projection has been developed and the corresponding transformation of the path integral measure was computed in a lattice regularization. The second supersymmetry of the $\mathrm{CP}^1 \cong \mathrm{O}(3)$ model was derived in terms of constrained field variables and the resulting expression allowed for a conclusive discussion of the possibility to construct a lattice discretization of the model which maintains both O(3) as well as a part of supersymmetry. The analysis how the symmetry transformations act on the field constraints revealed that such a construction is impossible. As a consequence, a manifestly O(3) symmetric discretization was chosen in order to perform explicit Monte Carlo computations with the aim to restore supersymmetry in the continuum limit. A stereographic projection has been applied in a second step, such that the algorithm could be implemented in terms of unconstrained variables. The degeneracy of fermionic and bosonic masses as well as a Ward identity for the bosonic action served as indicators for the restoration of supersymmetry. Explicit simulations showed that fine tuning is necessary, but already the introduction of a single mass parameter led to results which strongly indicate the restoration of supersymmetry in the continuum limit.

7. General Conclusion

Nonlinear sigma models have been established as a versatile tool to explore non-perturbative aspects of quantum field theories. While their structure is rich enough to provide descriptions of interesting phenomena in many areas of physics, they are well accessible to various analytic and numerical methods. They can therefore serve as ideal testing ground for conceptual investigations of different non-perturbative approaches to quantum field theory. Two of these approaches, lattice field theory and the Functional Renormalization Group (FRG), have been addressed in this thesis. They were studied in their application to nonlinear $\mathrm{O}(N)$ and CP^n models, which are employed as toy models or effective descriptions of many physical systems. Apart from being physically interesting, the numerous previous studies of these models offered useful benchmarks for the applied methods.
Although lattice field theory and the FRG have already been used for many years as complementary tools in field theory, only limited knowledge is available about a direct comparison of both approaches. For this purpose the renormalization flow of nonlinear $\mathrm{O}(N)$ models in three dimenions was examined by means of both approaches. The model is a particularly interesting testing ground with regard to the concept of non-perturbative renormalizability.
Starting with the FRG calculations, it was quickly realized that it becomes unfeasible to study the nonlinear model as a limit of the linear one, if one wants to study operators of higher orders. Instead, a manifestly nonlinear and covariant formulation of the model was employed to study an ansatz of the effective average action which includes all operators up to the fourth order in the derivatives. In order to find a reparametrization invariant formulation of the flow equation, a covariant background field expansion was applied. The beta functions could be extracted from this by means of off-diagonal heat kernel expansions. It was noticed that the introduction of the regulator inevitably leads to an action functional which depends separately on background and fluctuation fields. In order to account for this, a scaling parameter for the fluctations as well as a mass parameter were introduced.
The investigation of the flow equations showed that the nontrivial fixed point which was already detected in the simplest truncation remains stable if one includes two

of the three possible fourth order operators. These operators only add IR-irrelevant directions to the parameter space, and one of the couplings is identically zero at the fixed point. The second fourth order operator, however, renders the FRG computation sensitive to the N-dependence of the critical properties of the model, such that the critical exponent ν of the correlation length could be determined in qualitative agreement with the literature values. The inclusion of the mass term does not provide an improvement of the results and the impact of the scaling of the fluctuation field seems to be ambigious.

Despite these promising findings in the reduced truncation, no nontrivial fixed point could be identified in the full fourth order ansatz for the effective action. Further investigations are required to clearify if this lack of a fixed point is only a shortcoming of the limited truncation or if it points towards more subtle conceptual issues. One possible conceptual problem could be related to the treatment of the path integral measure in the FRG framework. Following arguments which suggest a regulator-dependent modification of the path integral measure, an additional term in flow equation was considered. Choosing an ansatz for the measure, the computations seem to stabilize and a nontrivial fixed point with only one relevant direction could be found for the full fourth order truncation. However, the critical exponents deviate strongly from the literature results. Therefore no final conclusion can be drawn, but further considerations are necessary about the appropriate definition of the path integral measure in nonlinear theories which are formulated in terms of a background field expansion.

After the renormalization flow was derived in the FRG framework, the Monte Carlo Renormalization Group (MCRG) was introduced as a possibility to determine flow diagrams in coupling space from computations in lattice field theory. The presented approach relies on block spin transformations on the lattice and the subsequent determination of renormalized couplings by means of a microcanonical demon method. Relating initial and renormalized couplings yields the beta functions as well as flow diagrams. The preliminary results for a full fourth order truncation confirm the existence of a nontrivial fixed point which has only one relevant direction and hence provide further evidence for the scenario of non-perturbative renormalizability. The results of MCRG and FRG agree qualitatively with each other and the quantitative deviations could be explained by differences in the regularization and truncation procedures. Having a numerical tool to compute flow diagrams, it would be interesting to draw further comparisons of both non-perturbative methods by applying them to other models.

The Average Effective Hamiltonian Action is a formulation of the FRG in phase space and has been recently proposed as an alternative approach to investigate the renormalization of theories. In this thesis applications to the nonlinear sigma model were considered in order to test this new ansatz. A Lorentz covariant formulation was used, although properties of its UV regularization have to be clearified further for the case of Hamiltonians which are more than quadratic in the momenta.

First, the consistency of this approach with the standard Lagrangian formulation was shown in simple truncations of the linear and nonlinear sigma model. Because operators of higher order in the canonical momenta are naturally generated in the Hamiltonian formulation of nonlinear sigma models, an expansion of the action functional in powers of momenta was considered. Such an expansion is not directly comparable to the usual derivative expansion, but provides an alternative access to the renormalization properties of the model. The nonlinear $\mathrm{O}(N)$ model was studied in detail and the flow equation was derived for a generic function of a covariant operator which is quadratic in the canonical momenta. The result was examined for a polynomial ansatz in three dimensions and a stable nontrivial fixed point with only one IR-relevant direction could be found at each order of the truncation. The corresponding critical exponent ν, however, does not show the correct dependence on N.

Finally, the FRG framework was used to address the subtle question of a possible renormalization of topological charges. The topological term of the two-dimensional $\mathrm{CP}^1 \cong \mathrm{O}(3)$ model was studied as the limit of a more general operator that contains an auxiliary field which is set constant at the end. The investigation of the UV was performed by means of a heat kernel expansion and a careful analysis of a coincidence limit and revealed that a possible running in the extreme UV is suppressed by the asymptotic freedom of the theory. The extreme IR had to be studied separately and a special representation of the Clifford algebra was constructed which made it possible to formulate the bosonic problem in terms of Dirac operators and to apply the index theorem. This analysis revealed a finite discrete renormalization of the topological charge due to zero modes. After similar findings in Yang-Mills and Chern-Simons theory, this result for the CP^1 model is a further indication that topological parameters may be renormalized due to effects in the extreme IR.

The last chapter of this thesis focussed on the lattice approach and in particular on the possibility to construct discretizations of supersymmetric field theories which maintain a part of the supersymmetry. The supersymmetric extension of the nonlinear $\mathrm{O}(3) \cong \mathrm{CP}^1$ model was studied for this purpose, because its target space is a Kähler manifold and the theory hence exhibits an additional supersymmetry. First, a supersymmetric version of the stereographic projection was developed and the corresponding Jacobian was computed, before an expression for the second supersymmetry was derived in terms of constrained field variables. A thorough analysis of both supersymmetry transformations and their action on a lattice discretization of the model showed that it is impossible to construct a lattice formulation of the theory which maintains the O(3) symmetry as well as a part of supersymmetry at finite lattice spacing. Thereafter, a manifestly O(3) symmetric discretization was chosen and Monte Carlo simulations were performed in order to investigate if the supersymmetry can be restored in the continuum limit. The measurement of the mass degenenarcy of bosons and fermions as well as a Ward identity suggest that this is indeed possible if only one parameter is fine tuned. Besides providing a non-perturbative method to investigate this specific supersymmetric model, the analysis also stressed the problem that the attempt to formulate a manifestly supersymmetric lattice action of some model can be in conflict with other symmetries of the considered theory.

This thesis illustrated that the well-established nonlinear sigma models still provide interesting insights into non-perturbative effects of quantum field theories. Besides the possibility to deepen the understanding of phenomena which are yet not fully understood, like supersymmetric field theories or topological charges, conceptual investigations of the lattice approach as well as of covariant and Hamiltonian formulations of the FRG could be performed.

A. Appendix

A.1. Two Alternative Formulations of a Fourth-Order Derivative Expansion

In order to determine the relation between the covariant (3.4) and the constrained formulation (3.53) of the fourth-order derivation expansion of the nonlinear $\mathrm{O}(N)$ model, one can choose stereographic coordinates (2.9) as examplary unconstrained parametrization of (3.4) and apply the inverse stereographic projection (2.11).
It is straigth forward to check that the bare action functionals of both formulations are equal up to a numerical factor

$$\frac{4}{(1+\boldsymbol{\phi}^2)^2}\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi} = \partial_\mu\boldsymbol{n}\partial^\mu\boldsymbol{n}\,, \tag{A.1}$$

such that $\zeta = \frac{g_1}{4}$. A similar, but a bit more tedious calculation yields the stereographic projection of

$$\begin{aligned}\partial^2\boldsymbol{n}\partial^2\boldsymbol{n} =& \frac{4\partial^2\boldsymbol{\phi}\partial^2\boldsymbol{\phi}}{(1+\boldsymbol{\phi}^2)^2} + \frac{16(\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi})^2}{(1+\boldsymbol{\phi}^2)^3} + \frac{16(\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi})(\boldsymbol{\phi}\partial^2\boldsymbol{\phi})}{(1+\boldsymbol{\phi}^2)^3} - \frac{32(\boldsymbol{\phi}\partial_\mu\boldsymbol{\phi})(\partial^\mu\boldsymbol{\phi}\partial^2\boldsymbol{\phi})}{(1+\boldsymbol{\phi}^2)^3}\\ &- \frac{64(\boldsymbol{\phi}\partial_\nu\boldsymbol{\phi})^2(\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi})}{(1+\boldsymbol{\phi}^2)^4} + \frac{64(\boldsymbol{\phi}\partial_\mu\boldsymbol{\phi})(\partial^\mu\boldsymbol{\phi}\partial^\nu\boldsymbol{\phi})(\boldsymbol{\phi}\partial_\nu\boldsymbol{\phi})}{(1+\boldsymbol{\phi}^2)^4}\end{aligned} \tag{A.2}$$

This expression looks quite complicated, but can be written in a compact way in terms of $\Box\phi^a$, which reads in stereographic coordinates

$$\Box\phi^a = \partial^2\phi^a + \frac{2}{1+\boldsymbol{\phi}^2}\left(\phi^a(\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi}) - 2\partial_\mu\phi^a(\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi})\right), \tag{A.3}$$

and leads to

$$h_{ab}\Box\varphi^a\Box\varphi^b = \tfrac{1}{4}(\partial^2\boldsymbol{n}\partial^2\boldsymbol{n}) - \frac{4}{(1+\boldsymbol{\phi}^2)^4}(\partial_\mu\boldsymbol{\phi}\partial^\mu\boldsymbol{\phi})^2 = \tfrac{1}{4}(\partial^2\boldsymbol{n}\partial^2\boldsymbol{n}) - \tfrac{1}{4}(\partial_\mu\boldsymbol{n}\partial^\mu\boldsymbol{n})^2. \tag{A.4}$$

The operators corresponding to the couplings L_1 and L_2 can be translated analogous to (A.1). The reformulation of the covariant action (3.4) in terms of constrained fields is finally given as

$$\begin{aligned}\mathcal{L}_{\text{eff}} =& \tfrac{1}{2}\,\zeta\, h_{ab}\partial_\mu\phi^a\partial^\mu\phi^b + \tfrac{1}{2}\,\alpha\, h_{ab}\Box\phi^a\Box\phi^b + \tfrac{1}{2}\,L_1(h_{ab}\partial_\mu\phi^a\partial_\nu\phi^b)^2 + \tfrac{1}{2}\,L_2(h_{ab}\partial_\mu\phi^a\partial^\mu\phi^b)^2\\ =& \tfrac{1}{2}\,\frac{\zeta}{4}\,\partial_\mu\boldsymbol{n}\partial^\mu\boldsymbol{n} + \tfrac{1}{2}\,\frac{\alpha}{4}\,\partial^2\boldsymbol{n}\partial^2\boldsymbol{n} + \tfrac{1}{2}\,\frac{L_1}{16}\,(\partial_\mu\boldsymbol{n}\partial_\nu\boldsymbol{n})^2 + \tfrac{1}{2}\,\frac{L_2-4\alpha}{16}\,(\partial_\mu\boldsymbol{n}\partial^\mu\boldsymbol{n})^2\,.\end{aligned} \tag{A.5}$$

A.2. Conventions and Fierz Identities

The two-dimensional Majorana representation used in Chap. 6 is given in terms of Pauli matrices as

$$\gamma_0 = \sigma_3, \quad \gamma_1 = -\sigma_1, \quad \gamma_* = \mathrm{i}\gamma_0\gamma_1 = \sigma_2\,. \quad C = -\mathrm{i}\sigma_2, \tag{A.6}$$

The conjugate spinor is defined as $\bar\chi = \chi^T C$ and fulfills the Fierz relation

$$\psi\bar\chi = -\tfrac{1}{2}\bar\chi\psi\mathbb{1} - \tfrac{1}{2}(\bar\chi\gamma^\mu\psi)\gamma_\mu - \tfrac{1}{2}(\bar\chi\gamma_*\psi)\gamma_*. \tag{A.7}$$

Due to the symmetry properties

$$\bar\chi\psi = \bar\psi\chi, \quad \bar\chi\gamma^\mu\psi = -\bar\psi\gamma^\mu\chi, \quad \bar\chi\gamma_*\psi = -\bar\psi\gamma_*\chi \tag{A.8}$$

the two last terms in (A.7) vanish for $\chi = \psi$ such that

$$\psi\bar\psi = -\tfrac{1}{2}\bar\psi\psi\,\mathbb{1}\,. \tag{A.9}$$

A.3. Invariance of the Nonlinear O(3) Action under the Second Supersymmetry

The invariance of the on-shell action

$$S[\boldsymbol{n},\boldsymbol{\psi}] = \int d^2x\;\partial_\mu\boldsymbol{n}\,\partial^\mu\boldsymbol{n} + \mathrm{i}\bar{\boldsymbol{\psi}}\not{\partial}\boldsymbol{\psi} + \tfrac{1}{4}(\bar{\boldsymbol{\psi}}\boldsymbol{\psi})^2 \tag{A.10}$$

under the second supersymmetry transformations (6.24) shall be proven here. The variation of the Lagrangian is[1]

$$\delta\mathcal{L} = 2\mathrm{i}\partial_\mu\boldsymbol{n}\cdot\partial^\mu(\boldsymbol{n}\times\bar\epsilon\boldsymbol{\psi}) - 2\mathrm{i}\bar{\boldsymbol{\psi}}\not{\partial}(\boldsymbol{n}\times\not{\partial}\boldsymbol{n}\epsilon) + 2\bar{\boldsymbol{\psi}}\not{\partial}(\bar\epsilon\boldsymbol{\psi}\times\boldsymbol{\psi}) - (\bar{\boldsymbol{\psi}}\boldsymbol{\psi})\,\bar{\boldsymbol{\psi}}(\boldsymbol{n}\times\not{\partial}\boldsymbol{n}\epsilon)\,. \tag{A.11}$$

[1] up to a negligible boundary term $\partial_\mu(-\bar{\boldsymbol{\psi}}\gamma^\mu(\bar\epsilon\boldsymbol{\psi}\times\boldsymbol{\psi}^\alpha))$

The term $\propto \boldsymbol{\psi}^5$ vanishes, since $\boldsymbol{\psi}$ is a Grassmannian field with only four independent degrees of freedom. It will be shown that the first and the second term in (A.11) cancel each other as well as the third and the fourth one. Starting with the first two terms, they can be written as

$$2\mathrm{i}\partial_\mu \boldsymbol{n}(\boldsymbol{n}\times\bar{\epsilon}\partial^\mu\boldsymbol{\psi}) - 2\mathrm{i}\bar{\boldsymbol{\psi}}(\boldsymbol{n}\times\partial^2\boldsymbol{n}\epsilon) - 2\mathrm{i}\bar{\boldsymbol{\psi}}\gamma^\mu\gamma^\nu\epsilon(\partial_\mu\boldsymbol{n}\times\partial_\nu\boldsymbol{n})\,. \tag{A.12}$$

The last term vanishes since $\partial_\mu\boldsymbol{n}\times\partial_\nu\boldsymbol{n}$ is parallel to $\boldsymbol{n}$ and hence perpendicular to $\boldsymbol{\psi}$. Integrating the second term by parts one sees that the first and second term cancel owing to the cyclicity of the triple product.

The cancellation of the third and fourth term in (A.11) is a bit more involved. First, one partially integrates the third term and obtains $-2\partial_\mu\bar{\boldsymbol{\psi}}\gamma^\mu(\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi})$. Since $\boldsymbol{n}\boldsymbol{\psi}^\alpha = 0$ for both spinor components α, it follows that $\bar{\epsilon}\bar{\boldsymbol{\psi}}\times\boldsymbol{\psi}$ is parallel to $\boldsymbol{n}$ such that

$$-2\partial_\mu\bar{\boldsymbol{\psi}}\gamma^\mu(\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi}) = -2(\partial_\mu\bar{\boldsymbol{\psi}}\gamma^\mu\boldsymbol{n})\;\boldsymbol{n}(\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi})\,. \tag{A.13}$$

The condition $\bar{\boldsymbol{\psi}}\boldsymbol{n} = 0$ implies $\partial_\mu\bar{\boldsymbol{\psi}}\boldsymbol{n} = -\bar{\boldsymbol{\psi}}\partial_\mu\boldsymbol{n}$. (A.13) can hence be written as $2(\bar{\boldsymbol{\psi}}\not{\partial}\boldsymbol{n})\;\boldsymbol{n}(\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi})$. To proceed further, one utilizes $\bar{\psi}_1 n_1 = -\bar{\psi}_2 n_2 - \bar{\psi}_3 n_3$ and the Fierz relation $\bar{\psi}_i\gamma^\mu\psi_i = 0$:

$$\begin{aligned}&2(\bar{\psi}_1\not{\partial}n_1 + \bar{\psi}_2\not{\partial}n_2 + \bar{\psi}_3\not{\partial}n_3)\big[n_1\bar{\epsilon}\psi_2\cdot\psi_3 - n_1\bar{\epsilon}\psi_3\cdot\psi_2 + \text{cyclic terms}\big] \\ &= 2\bar{\psi}_2\gamma^\mu\psi_3\big(\partial_\mu n_2\cdot n_1 - \partial_\mu n_1\cdot n_2\big)\bar{\epsilon}\psi_2 + 2\bar{\psi}_3\gamma^\mu\psi_2\big(\partial_\mu n_1\cdot n_3 - \partial_\mu n_3\cdot n_1\big)\bar{\epsilon}\psi_3 + \text{c. t}\,.\end{aligned} \tag{A.14}$$

The Fierz relation $(\bar{\alpha}\gamma^\mu\beta)\,\bar{\epsilon}\alpha = \frac{1}{2}\bar{\alpha}\alpha\,(\bar{\beta}\gamma^\mu\epsilon)$ can be employed, which holds for Majorana spinors, and one obtains

$$(\bar{\psi}_2\psi_2)\bar{\psi}_3\gamma^\mu\epsilon(n_1\partial_\mu n_2 - n_2\partial_\mu n_1) + (\bar{\psi}_3\psi_3)\bar{\psi}_2\gamma^\mu\epsilon(n_3\partial_\mu n_1 - n_1\partial_\mu n_3) + \text{cyclic terms}\,.$$

Finally, using $(\bar{\alpha}\alpha)\bar{\alpha} = 0$ the third term in (A.11) can be written as

$$(\bar{\boldsymbol{\psi}}\boldsymbol{\psi})\;\bar{\boldsymbol{\psi}}(\boldsymbol{n}\times\not{\partial}\boldsymbol{n}\epsilon)\,. \tag{A.15}$$

As a result, the third and fourth term in (A.11) cancel each other. This proves that the action is invariant under the second supersymmetry transformation (6.24).

The invariance of the constraints can be shown easily:

$$\begin{aligned}\delta(\boldsymbol{n}^2) &= 2\mathrm{i}\boldsymbol{n}\cdot(\boldsymbol{n}\times\bar{\epsilon}\boldsymbol{\psi}) = 0 \\ \delta(\boldsymbol{n}\cdot\boldsymbol{\psi}) &= \mathrm{i}(\boldsymbol{n}\times\bar{\epsilon}\boldsymbol{\psi})\cdot\boldsymbol{\psi} - \boldsymbol{n}\cdot(\boldsymbol{n}\times\not{\partial}\boldsymbol{n}\epsilon) - \mathrm{i}\boldsymbol{n}\cdot(\bar{\epsilon}\boldsymbol{\psi}\times\boldsymbol{\psi}) = 0\,.\end{aligned}$$

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Zusammenfassung

Das Ziel dieser Arbeit war die Untersuchung und Weiterentwicklung von nicht-störungstheoretischen Methoden der Quantenfeldtheorie anhand ihrer Anwendung auf nichtlineare Sigma-Modelle.
Während ein großer Teil der physikalischen Phänomene der Quantenfeldtheorie durch die Störungstheorie erfolgreich vorhergesagt werden können, sind manche Aspekte im Bereich großer Kopplungsstärken noch nicht endgültig verstanden und bedürfen geeigneter nicht-störungstheoretischer Methoden zur ihrer Analyse. Diese Arbeit hat sich auf zwei Ansätze konzentriert, die numerische Behandlung von Feldtheorien auf diskretisierten Raumzeitgittern und die Funktionale Renormierungsgruppe (FRG) als Beschreibung des Renormierungsflusses von effektiven Wirkungen. Betrachtungen der nichtlinearen $\mathrm{O}(N)$ Modelle haben gezeigt, dass zur korrekten Analyse der kritischen Eigenschaften im Rahmen der FRG ein Ansatz gewählt werden muss, der vierte Ableitungsordungen enthält. Hierfür wurde ein kovarianter Formalismus entwickelt, der auf einer Hintergrundfeldentwickung und der Entwicklung eines Wärmeleitungskerns beruht. Abgesehen von einer destabilsierenden Kopplung deuten die Ergebnisse auf einen nichttrivialen Fixpunkt und damit auf die nicht-störungstheoretische Renormierbarkeit dieser Modelle hin. Die resultierenden Flussdiagramme wurden schließlich noch mit den Ergebnissen einer numerischen Analyse des Renormierungsflusses mithilfe der Monte Carlo Renormierungsgruppe verglichen und es wurde hierbei qualitative Übereinstimmung gefunden.
Desweiteren wurde eine alternative Formulierung der FRG in Phasenraumkoordinaten untersucht und ihre Konsistenz an einfachen Beispielen getestet. Darüber hinaus wurde eine alternative Entwicklung der effektiven Wirkung in Ordnungen der kanonischen Impulse auf die nichtlinearen $\mathrm{O}(N)$ Modelle angewandt, mit dem Ergebnis eines stabilen nichttrivialen Fixpunktes dessen kritischen Eigenschaften jedoch nicht die erwartete N-Abhängigkeit zeigen.
Mithilfe der FRG wurde schließlich noch die Renormierung topologischer Operatoren anhand der Windungszahl des $\mathrm{O}(3) \cong \mathrm{CP}^1$-Modells untersucht. Durch die Verallgemeinerung des topologischen Operators und die Entwicklung und Anwendung einiger eleganter mathematischen Methoden konnten Hinweise auf einen diskreten Sprung des topologischen Parameter im extrem Infraroten gefunden werden.
Abschließend wurde die supersymmetrische Erweiterung des $\mathrm{O}(3) \cong \mathrm{CP}^1$-Modells betrachtet im Hinblick auf die Möglichkeit derartige Theorien mit erweiterter Supersymmetrie auf einem Raumzeitgitter so zu diskretisieren, dass zumindest ein Teil der Supersymmetrie nicht gebrochen ist. Es konnte gezeigt werden, dass dies prinzipiell nicht möglich ist ohne dabei gleichzeitig die $\mathrm{O}(3)$-Symmetrie zu brechen.

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Ehrenwörtliche Erklärung

Ich erkläre hiermit ehrenwörtlich, dass ich die vorliegende Arbeit selbständig, ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel und Literatur angefertigt habe. Die aus anderen Quellen direkt oder indirekt übernommenen Daten und Konzepte sind unter Angabe der Quelle gekennzeichnet. Ergebnisse, die in Zusammenarbeit mit Mitarbeitern des Theoretisch-Physikalischen Institutes in Jena oder in anderen Kooperationen entstanden sind, sind in der Arbeit entsprechend benannt. Weitere Personen waren an der inhaltlich-materiellen Erstellung der vorliegenden Arbeit nicht beteiligt. Insbesondere habe ich hierfür nicht die entgeltliche Hilfe von Vermittlungs- bzw. Beratungsdiensten (Promotionsberater oder andere Personen) in Anspruch genommen. Niemand hat von mir unmittelbar oder mittelbar geldwerte Leistungen für Arbeiten erhalten, die im Zusammenhang mit dem Inhalt der vorgelegten Dissertation stehen. Die Arbeit wurde bisher weder im In- noch im Ausland in gleicher oder ähnlicher Form einer anderen Prüfungsbehörde vorgelegt. Die geltende Promotionsordnung der Physikalisch-Astronomischen Fakultät ist mir bekannt. Ich versichere ehrenwörtlich, dass ich nach bestem Wissen die reine Wahrheit gesagt und nichts verschwiegen habe.

Jena, den 31. August 2012

(Raphael Flore)

Lebenslauf

Name	Raphael Flore
geboren	am 21. Februar 1986 in Warburg (NRW)

Schule

1992-1996	J. D. Falk-Grundschule Warburg
1996-2005	Hüffertgymnasium Warburg
2005	Abitur

Studium

10/2005 - 09/2008	Diplomstudium Physik, Universität Göttingen
10/2008 - 09/2009	M.Sc. course Elementary Particle Theory, University of Durham
09/2009	Abschluss als Master of Science in Elementary Particle Theory
seit 11/2009	Doktorand am TPI Jena

Jena, den 31. August 2012

(Raphael Flore)