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COMPUTATION OF EFFECTIVE HAMILTONIANS BY MONTE CARLO SIMULATIONS WITH FIXED BLOCK SPINS

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Abstract. A Monte Carlo method for the computation of effective Hamiltonians for classical spin systems on a lattice is presented. The procedure is based on Monte Carlo simulations of auxiliary statistical mechanical systems with fixed block spins and thus avoids the simulation of systems with large or infinite correlation length. Effective Hamiltonians for arbitrary block spin configurations $\bar{\phi}$ as well as coefficients of a Taylor expansion about such configurations can be computed. The method allows a careful investigation of locality properties of the effective Hamiltonian. Results of Monte Carlo studies for two-dimensional spin models with block spins of fluctuating length are presented. One finds good agreement with second order high temperature expansions of the effective potential for a remarkably large range of the coupling constant.

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Introduction

The formulation of a quantum field theory as a Euclidean field theory on a lattice allows a study of nonperturbative phenomena (for example quark confinement in Quantum Chromodynamics [*1*]) and (in principle) provides the possibility of computing the mass spectrum from a few fundamental parameters. Euclidean lattice field theories can be investigated by the usual methods of classical statistical mechanics (e.g. Mayer expansions) or by Monte Carlo simulations [*29*].

In order to obtain physical results the lattice cutoff has to be removed (continuum limit).[1] A lattice field theory can exhibit continuum behaviour only if the correlation length diverges. In order to study the continuum limit it is therefore necessary to control statistical mechanical systems in the neighbourhood of a critical point. A framework for a systematic approach to this problem is Wilson's *renormalization group* [*2,3*].

The central idea of the renormalization group is to divide the problem of solving a theory with large or infinite correlation length into a sequence of "manageable problems". Starting from the fundamental Hamiltonian[2] $\mathcal{H}(\varphi)$ for "spins" φ on a lattice Λ with lattice spacing a, by successive *renormalization group transformations* one determines a sequence of *effective Hamiltonians* $\mathcal{H}_{\mathrm{eff}}^{(i)}(\phi^{(i)})$ for block spins $\phi^{(i)}$ which are defined on block lattices $\Lambda^{(i)}$ with lattice spacings $L^i a$. $L \geq 2$ is an integer scale factor. A renormalization group transformation preserves the partition function and does not change the long distance behaviour of the system. The correlation length in units of the lattice spacing is reduced by a factor of L. The correlation length of a critical theory remains infinite. A central assumption in renormalization group theory is that the (discrete) flow of effective Hamiltonians of a critical theory converges to a *renormalization group fixed point* $\mathcal{H}_{\mathrm{eff}}^{*}$. The renormalization group flow in the neighbourhood of the fixed point determines the critical properties of the theory (critical exponents, β-function).

The renormalization group method will be successful only if a single renormalization group transformation is easier to control than the full partition function. A renormalization group step is associated with an auxiliary statistical mechanical system whose partition function is the effective Boltzmannian $\exp[-\mathcal{H}_{\mathrm{eff}}(\phi)]$. In this auxiliary system integration is not over the full range of degrees of freedom but over "fluctuation fields" which have a propagator with an IR-cutoff in addition to the lattice UV-cutoff. It is a central ingredient of Wilson's "renormalization group philosophy" that the auxiliary system has short range correlations only (of order one block lattice spacing), even if the original theory has large or infinite correlation length. An equivalent assumption is that the effective Hamiltonian has good locality properties. For special systems (weakly coupled theories without spontaneous symmetry breaking) the validity of these assumptions was proven rigorously. An essential condition is a good choice of the block spin. Examples show that a "bad" block spin definition leads to dangerous nonlocalities of the effective Hamiltonian and qualitatively wrong results [*8, Remark C*]. Analytical renormalization group studies for weakly coupled theories [*18*] further show that the effective Hamiltonian has good locality properties to each order of perturbation theory. However, beyond perturbation theory there is a *large field problem*.

[1] It is not clear a priori that a non-trivial continuum theory exists. For example little doubt exists that the lattice cutoff of 4-dimensional φ^4 theory can only be removed if simultaneously the renormalized coupling constant is tuned to zero [*16 and references cited therein*].

[2] *Action* in Euclidean quantum field theory

For a given block spin configuration ϕ the lattice can contain *large field islands*[1], where the energy density is large. Within the islands long range correlations can occur. In weakly coupled theories the large field problem can be controlled, because in a generic (i.e. typical) block spin configuration large field islands which contain more than a few points are dilute, i.e. are very unlikely to occur..

At present analytical renormalization group techniques do not work for strongly coupled theories[2]. To investigate these models one can combine the renormalization group approach with the Monte Carlo method. This idea is due to S.K. Ma [32] and has been developed into a powerful method *(Monte Carlo Renormalization Group = MCRG)* [33-38] in the last ten years. However, most of the MCRG procedures do not take advantage of the central idea of the renormalization group: The Monte Carlo simulations are performed for the full theory with large or infinite correlation length.[3] Simulations of critical or nearly critical systems however suffer from *critical slowing down* and large *finite size effects*.[4]

In this paper a method is described for the computation of effective Hamiltonians which is close in spirit to Wilson's renormalization group philosophy. The method is based on "Monte Carlo simulations with fixed block spins". Simulations are not performed for the full theory but in the auxiliary statistical mechanical system with partition function $\exp[-\mathcal{H}_{\text{eff}}(\phi)]$. Following Wilson's hypothesis one can hope that such simulations do not suffer from critical slowing down and large finite size effects, at least in the small field region.

The computation of effective Hamiltonians by Monte Carlo simulations with fixed block spins had already been proposed by S.K. Ma in 1976 [32]. In his Cargèse Lectures 1983 Wilson writes [35]: *"A direct computation of the effective interactions $\mathcal{H}_i$ by Monte Carlo methods (as originally proposed by S.K. Ma) looks at first sight pretty hopeless. A separate Monte Carlo computation is required for each configuration of the block spins $\{t_m\}$. As many configurations need to be looked at as there are parameters in $\mathcal{H}_i[t]$ to be determined. There might be thousands or even millions of parameters in $\mathcal{H}_i[t]$ that are important. ... However, there remains a possibility that the number of important parameters in $\mathcal{H}_i$ might be held within reasonable bounds and that direct computations of the $\mathcal{H}_i$ might some day be feasible."*

It will be shown in this paper that the situation is not hopeless. By a Monte Carlo simulation with a single block spin configuration $\bar{\phi}$ it is possible to compute coefficients of a Taylor expansion for $\mathcal{H}_{\text{eff}}(\phi)$ about $\phi = \bar{\phi}$. Therefore a single Monte Carlo simulation allows a determination of many coupling constants simultaneously. For weakly coupled theories it can be proven rigorously that the effective Hamiltonian is an analytic function of the block spin variables in the small field region [18]. Thus in this region convergent and local Taylor expansions exist. It is expected that this remains true for strongly coupled theories.

The paper starts with a short introduction to the notions of the renormalization group and MCRG (Chapter I).

[1] The name *large field* is merely historical. Large fields are not necessarily large by value.

[2] Examples: A ferromagnet at the Curie point, φ^4 theory with large quartic coupling constant.

[3] Exceptions are the Callaway and Petronzio method [39], Gupta's *Improved MCRG* [40] and recent papers on the computation of the effective potential for φ^4 theory [41].

[4] Some MCRG procedures allow a systematic reduction of *finite size effects*, see Chapter I.

In Chapter II a first possibility of computing the effective Hamiltonian is discussed. The derivative of $\mathcal{H}_{\text{eff}}(\phi)$ with respect to the inverse temperature β is the expectation value of the fundamental Hamiltonian in an auxiliary statistical mechanical system with fixed block spins. By Monte Carlo simulations of this system one can compute $(\partial/\partial\beta)\mathcal{H}_{\text{eff}}(\phi)$ for arbitrary block spin configurations. $\mathcal{H}_{\text{eff}}(\phi)$ is then determined by integration over β. For this procedure Wilson's objection is valid: Monte Carlo simulations for many different block spin configurations have to be performed. However, it will be shown that the method is well suited for computing the effective potential (= effective Hamiltonian per volume for constant block spin). The Monte Carlo procedure is described in some detail for the O(N) symmetric nonlinear σ-model. In contrast to MCRG studies for these spin models in the literature [36-38], a linear block spin definition is used: the block spins are defined as block averages of the fundamental spins ("block spins of fluctuating length"). To generate spin configurations with fixed block averages an algorithm is proposed which simultaneously updates pairs of spins belonging to the same block. Monte Carlo results for the effective potential of the 2-dimensional Ising model and the 2-dimensional O(3) model are presented. The results agree with the expected qualitative picture of the renormalization group flow. For the Ising model a fixed point is found, with critical exponents ν and η consistent with their exactly known values. For the O(3) model with increasing block size, transitions from potentials with a double well shape to such with minimum at $\phi = 0$ take place. The results of the Monte Carlo simulations are compared with $O(\beta^2)$ high temperature expansions. A remarkably good agreement is found up to the critical point for the Ising model and for the O(3) model up to β-values where the correlation length is very large. This is an impressive confirmation of the meaning of Wilson's hypothesis that the effective Hamiltonian is the free energy of a noncritical auxiliary statistical mechanical system if the block size is not too large. For such noncritical systems high temperature expansions have a chance to produce good approximations.

For a linear *Gaussian* block spin transformation the relation of locality properties of the effective Hamiltonian and properties of the auxiliary system is very transparent (Chapter III). The kernels of a Taylor expansion for $\mathcal{H}_{\text{eff}}(\phi)$ about $\phi = \bar{\phi}$ are truncated correlation functions of block averages of the spins in the auxiliary system with partition function $\exp[-\mathcal{H}_{\text{eff}}(\bar{\phi})]$. Monte Carlo simulations of this system are easy to do. Since the block averages of the spins may fluctuate away from the fixed block spins, a Monte Carlo procedure can be used which updates single spins. Monte Carlo results for the 2-dimensional Ising model at the critical point are presented. The results clearly indicate a large field problem. Regions of the lattice where $\phi \approx 0$ belong to large field islands. One finds that Taylor kernels of the effective Hamiltonian for this model do not have good locality properties if the expansion is about $\bar{\phi} = 0$.

In Chapter IV a Monte Carlo procedure for the computation of Taylor expansions for the effective Hamiltonian of φ^4 theory is described. The Taylor coefficients of an expansion about $\phi = \bar{\phi}$ can be expressed as truncated correlation functions in the auxiliary system with fixed block spins $\bar{\phi}$. The method therefore allows a careful investigation of locality properties of Taylor expansions about arbitrary reference configurations $\bar{\phi}$, especially in the large field region.

The paper is concluded with a short summary and some remarks on possible future applications of the method.

Chapter I

Wilson's Renormalization Group and MCRG

The basic notions of Wilson's renormalization group are introduced, and the idea of standard MCRG (Monte Carlo Renormalization Group) is explained.

Euclidean lattice field theories can be looked at as systems of classical statistical mechanics with random variables (spins) defined on the sites of a cubic lattice.[1] Thus one has a d-dimensional lattice $\Lambda \subseteq (aZ)^d$ and fields $\underline{\varphi} : \Lambda \to Q$, $z \to \underline{\varphi}(z)$. a denotes the lattice spacing. Examples for Q are: Q = real numbers in scalar field theory, $Q = \pm 1$ for the Ising model, Q = unit sphere S^{N-1} for O(N) nonlinear σ-models, Q = SU(N) in pure lattice gauge theory.

We consider canonical ensembles with partition functions

$$Z = \int \prod_{z \in \Lambda} d\underline{\varphi}(z)\, e^{-\mathcal{H}(\underline{\varphi})} \tag{1}$$

$d\underline{\varphi}(z)$ denotes a measure on Q, e.g. the Lebesgue measure for real variables, the invariant Z_2 summation for Ising variables, the uniform measure on S^{N-1} for Heisenberg spins, the invariant Haar measure on SU(N) for gauge variables. Let us abbreviate $\mathcal{D}\underline{\varphi} \equiv \prod_{z \in \Lambda} d\underline{\varphi}(z)$.

The probability distribution of the fields $\underline{\varphi}$ is determined by the Hamiltonian $\mathcal{H}(\underline{\varphi})$. An example is the Hamiltonian of scalar $\underline{\varphi}^4$ theory:

$$\mathcal{H}(\underline{\varphi}) = \frac{1}{2} \int_{z \in \Lambda} \underline{\varphi}(z)[-\Delta \underline{\varphi}](z) + \frac{m_0^2}{2} \int_{z \in \Lambda} \underline{\varphi}(z)^2 + \frac{\lambda_0}{4!} \int_{z \in \Lambda} \underline{\varphi}(z)^4 \tag{2}$$

Integrals on the lattice are Riemannian sums: $\int_{z \in \Lambda} f(z) \equiv \sum_{z \in \Lambda} a^d f(z)$. The lattice Laplacian is defined by

$$(\Delta \underline{\varphi})(z) = a^{-2} \sum_{\mu=1}^{d} [\underline{\varphi}(z + a\hat{\mu}) + \underline{\varphi}(z - a\hat{\mu}) - 2\underline{\varphi}(z)] \tag{3}$$

$\hat{\mu}$ denotes the unit vector in μ-direction.

The fields $\underline{\varphi}$ have a dimension. With the exception of this chapter we will use dimensionless fields φ. For a representation on a computer this is necessary. The relation of $\underline{\varphi}$ and φ is given by $\underline{\varphi}(z) \equiv a^{\frac{1}{2}(2-d)} \varphi(z)$.

Expectation values of observables are defined by

$$\langle \mathcal{O}(\underline{\varphi}) \rangle \equiv Z^{-1} \int \mathcal{D}\underline{\varphi}\, e^{-\mathcal{H}(\underline{\varphi})}\, \mathcal{O}(\underline{\varphi}) \tag{4}$$

[1] The random variables of a pure lattice gauge theory live on links which connect nearest neighbours in the lattice.

An (exact) renormalization group transformation (block spin transformation) maps a lattice field theory on a lattice Λ (lattice spacing a) to an effective lattice field theory which is defined on a block lattice Λ' with lattice spacing $a' \equiv L \cdot a$, $L \geq 2$, integer. The effective theory has an UV-cutoff which is smaller by a factor of L. The transformation affects the Hamiltonian and the observables; eventually the type of the fields is changed. However, the partition function and expectation values of (suitably transformed) observables remain unchanged.

It is the idea of the renormalization group to summarize the effect of fluctuations over length scales which are smaller than a certain scale factor L in an effective theory for block spin variables $\underline{\phi}(x)$. The choice of a block spin definition is not unique.[1] A natural block spin definition is to take as block spins the averages of the original fields $\underline{\varphi}$ over cubic blocks with side length L. Λ is divided into cubic blocks of size L^d. Each of these blocks corresponds to a site x of the block lattice Λ'. As block lattice sites one might choose the centers of the blocks (see Figure I.1.). Λ' is again a cubic lattice, with lattice spacing $a' = L \cdot a$.

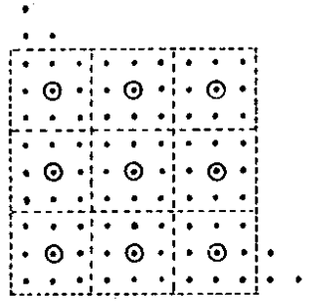

Figure I.1. A section of a 2-dimensional lattice Λ. The blocks consist of 3×3 sites $z \in \Lambda$, i.e. $L = 3$. The block centers are identified with the sites x of the block lattice Λ'.

For $x \in \Lambda'$ one defines

$$\underline{\phi}(x) \equiv L^{-d} \sum_{z \in x} \underline{\varphi}(z) \equiv \underset{z \in x}{\mathrm{av}}\, \underline{\varphi}(z) \tag{5}$$

This is a linear block spin definition. Linear renormalization group transformations can lead to block spin variables which are not of the same type as the fields of the original theory. If the fundamental fields are spins of unit length (Heisenberg ferromagnet) then this is not true for the block averages: The block variables are "spins of fluctuating length". In this paper only linear block spin transformations will be used.

[1] A "bad" choice of the block spin might lead into a disaster, see the corresponding remark in the Introduction.

As an example for a nonlinear block spin definition let us consider the so called *majority rule* for the Ising model. One puts $\phi(x) = +1$ if a majority of spins in block x has value $+1$. In the other case the block spin is $\phi(x) = -1$. If the number of spins in the block is even a zero block average can occur. In this case $\phi(x) = \pm 1$ is selected with equal probability.

If one wants to define dimensionless block spin fields one has to take into account that the yard stick on the block lattice is given by the block lattice spacing a'. Dimensionless block spins $\underline{\phi}$ are thus defined by $\underline{\phi}(x) \equiv (a')^{\frac{1}{2}(2-d)}\phi(x)$. For dimensionless fields the linear block spin definition reads

$$\phi(x) = L^{\frac{1}{2}(d-2)} \operatorname*{av}_{z \in x} \varphi(z) \tag{6}$$

Eventually in addition to the factor $L^{\frac{1}{2}(d-2)}$ an *anomalous dimension* has to be taken into account (wave function renormalization). We will come back to this later.

The *effective Hamiltonian* $\mathcal{H}_{\text{eff}}(\underline{\phi})$ determines the probability distribution of the block spins $\underline{\phi}(x)$ on the block lattice Λ'. It is natural to require that the probability distribution for $\underline{\phi}$ should be exactly the same as the distribution of the corresponding block averages in the original theory. This guarantees that correlation functions of the fundamental spins at distances which are large compared with the block length L can be expressed in a simple way in terms of correlation functions of the block spins. This in mind one is led to the following definition:

$$e^{-\mathcal{H}_{\text{eff}}(\underline{\phi})} = \int \mathcal{D}\underline{\varphi}\, e^{-\mathcal{H}(\underline{\varphi})} \prod_{x \in \Lambda'} \delta[\underline{\phi}(x) - \operatorname*{av}_{z \in x} \underline{\varphi}(z)] \equiv \mathcal{Z}(\underline{\phi}) \tag{7}$$

$\mathcal{Z}(\underline{\phi}) = e^{-\mathcal{H}_{\text{eff}}(\underline{\phi})}$ is called *effective Boltzmannian*. It is easy to verify that integration of $\mathcal{Z}(\underline{\phi})$ over the block spin variables $\underline{\phi}$ yields again the partition function.

The conservation of the partition function is essential for the fact that the system does not change its thermodynamical properties when a block spin transformation is applied. A general class of renormalization group transformations which have this property can be written in the form

$$e^{-\mathcal{H}_{\text{eff}}(\underline{\phi})} \equiv \int \mathcal{D}\underline{\varphi}\, P(\underline{\phi}|\underline{\varphi}) e^{-\mathcal{H}(\underline{\varphi})} \tag{8}$$

with a kernel $P(\underline{\phi}|\underline{\varphi}) \geq 0$ which obeys $\int \mathcal{D}\underline{\phi}\, P(\underline{\phi}|\underline{\varphi}) = 1$.

The kernel of the transformation defined by Eq. (7) is

$$P(\underline{\phi}|\underline{\varphi}) = \prod_{x \in \Lambda'} \delta[\underline{\phi}(x) - \operatorname*{av}_{z \in x} \underline{\varphi}(z)] \tag{9}$$

In Chapter III we will use Gaussian block spins:

$$P(\underline{\phi}|\underline{\varphi}) = \mathcal{N}_\kappa^{-1} \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa[\underline{\phi}(x) - \operatorname{av}_{z \in x} \underline{\varphi}(z)]^2} \tag{10}$$

The normalization factor $\mathcal{N}_\kappa$ has to be chosen such that integration over the $\underline{\phi}$-variables yields one. Details on Gaussian block spins can be found in Chapter III and in Appendix B.1.

Renormalization group transformations can be iterated. This leads to a sequence of effective Hamiltonians $\mathcal{H}_{\text{eff}}^{(i)}(\phi^{(i)})$ for block spins $\phi^{(i)}$ on block lattices $\Lambda^{(i)}$ with lattice spacings $a_i \equiv L^i a$. We write $\mathcal{H}_{\text{eff}}^{(i+1)} = \mathcal{R}[\mathcal{H}_{\text{eff}}^{(i)}]$. For linear block spin transformations with δ prescription two successive block spin transformations with scale factors L_1 and L_2 can be replaced by a single transformation with a scale factor $L_1 \cdot L_2$. This follows from the fact that the average of an average is again an average. The composition rules for Gaussian block spin transformations are a little bit more complicated: The composition of two Gaussian distributions is again Gaussian but with a modified "width" (see Appendix B.1.).

In this paper advantage will be taken of the fact that iterated renormalization group transformations can be replaced by a single transformation with large block size. However, the blocks must not be chosen too big, otherwise a renormalization group step can become an unmanageable problem.

For the block spin definition Eq. (9) spatial averages of correlation functions in the fundamental theory can be expressed in terms of corresponding correlation functions in the effective theory, for example

$$\operatorname*{av}_{v \in x} \operatorname*{av}_{w \in y} \langle \underline{\varphi}(v)\underline{\varphi}(w)\rangle_{\mathcal{H}} = \langle \underline{\phi}(x)\underline{\phi}(y)\rangle_{\mathcal{H}_{\text{eff}}} \tag{11}$$

If the distance $|x - y|$ is large compared with the block size the L^{2d} contributions on the left hand side are approximately equal, and

$$\langle \underline{\varphi}(v)\underline{\varphi}(w)\rangle_{\mathcal{H}} \approx \langle \underline{\phi}(x)\underline{\phi}(y)\rangle_{\mathcal{H}_{\text{eff}}} \tag{12}$$

for $v \in x$ and $w \in y$. The *effective observables* for n-point functions at large distances are therefore of a simple form. For arbitrary observables $\mathcal{O}(\underline{\varphi})$ effective observables $\mathcal{O}_{\text{eff}}(\underline{\phi})$ can be defined such that

$$\langle \mathcal{O}(\underline{\varphi})\rangle_{\mathcal{H}} = \langle \mathcal{O}_{\text{eff}}(\underline{\phi})\rangle_{\mathcal{H}_{\text{eff}}} \tag{13}$$

This is achieved by

$$\mathcal{O}_{\text{eff}}(\underline{\phi})\, e^{-\mathcal{H}_{\text{eff}}(\underline{\phi})} \equiv \int \mathcal{D}\underline{\varphi}\, e^{-\mathcal{H}(\underline{\varphi})} \mathcal{O}(\underline{\varphi}) \prod_{x \in \Lambda'} \delta[\underline{\phi}(x) - \operatorname*{av}_{z \in x} \underline{\varphi}(z)] \tag{14}$$

Renormalization group transformations do not change the correlation length of a theory. As a consequence the correlation length in units of the actual lattice spacing will be reduced by a factor of L. Of course, an infinite correlation length remains infinite. It is a central assumption of the renormalization group that the flow of effective Hamiltonians of a *critical* theory converges to a renormalization group fixed point $\mathcal{H}_{\text{eff}}^*$. A renormalization group fixed point is defined by $\mathcal{R}[\mathcal{H}_{\text{eff}}^*] = \mathcal{H}_{\text{eff}}^*$.[1]

[1] The existence of a renormalization group fixed point is equivalent to scale invariance at large distances, see also Figure 1.2. at the end of this chapter.

For a linear block spin transformation a fixed point in general can exist only if a wave function renormalization is taken into account in the block spin definition such that

$$\underline{\phi}(x) = f^{-\frac{1}{2}} \underset{z \in x}{\text{av}} \underline{\varphi}(z) \tag{15}$$

Close to a fixed point the renormalization constant f is related to the critical exponent η. For the 2-point function at a fixed point and for large x:

$$G^*(x) \equiv \langle \phi(0)\phi(x) \rangle_{\mathcal{H}^*_{\text{eff}}} \approx L^{d-2} f^{-1} \langle \phi(0)\phi(Lx) \rangle_{\mathcal{H}^*_{\text{eff}}} = L^{d-2} f^{-1} G^*(Lx) \tag{16}$$

For positive g the functional equation $f(\lambda x) = g(\lambda) f(x)$ has the unique solution $g(\lambda) = \lambda^r$ and $f(x) = \text{const} \cdot x^r$. r must be real. Thus

$$\begin{aligned} G^*(x) &\propto |x|^{r} \\ L^{2-d} f &= L^r \end{aligned} \tag{17}$$

We have thus shown that the existence of a renormalization group fixed point implies that the 2-point function of a critical theory decays according to a power law. A critical exponent η is usually defined (see for example [2]) by

$$G^*(x) \propto |x|^{-(d-2+\eta)} \tag{18}$$

Thus the relation of the constant f and the anomalous dimension η at a renormalization group fixed point is given by $f^{-1} = L^\eta$.

The *Monte Carlo renormalization group* is based on work of Ma [32] and Kadanoff [33]. Essential contributions are due to Wilson [34], Swendsen [36] and Shenker and Tobochnik [37]. There is a lot of literature on MCRG. A small number of papers is cited in the "References".

Though there are many MCRG methods and tricks, some of them designed for special models, the basic idea of MCRG is relatively simple:

By Monte Carlo simulation of the original theory one generates a sequence of φ-configurations on a lattice $\Lambda \equiv \Lambda^{(0)}$ with a probability distribution determined by the fundamental Hamiltonian $\mathcal{H}(\varphi)$. For each of these configurations $\varphi \equiv \phi^{(0)}$ block spin configurations $\phi^{(i)}$, $i \geq 1$, are generated according to the probability measure

$$\text{dprob}[\phi^{(i+1)}] \propto \prod_{x \in \Lambda^{(i+1)}} d\phi^{(i+1)}(x)\, P(\phi^{(i+1)} | \phi^{(i)}) \tag{19}$$

In the case of the δ block spin $\phi^{(i+1)}$ is uniquely determined by $\phi^{(i)}$ (e.g. as block average). However, in general the block spins will depend on the fundamental spins in a probabilistic way, and one has to generate the actual block spin configuration by some stochastic procedure. (Of course the number of possible block spin transformations that can be performed is limited by the size of the finest lattice $\Lambda^{(0)}$.) It is easy to see that in this way on each of the lattices $\Lambda^{(i)}$ one obtains a sequence of configurations which are distributed exactly according to the

effective Hamiltonian $\mathcal{H}^{(i)}_{\text{eff}}(\phi^{(i)})$. Thus expectation values of observables of the block spin fields can directly be computed as averages over the "blocked" Monte Carlo sequence of fundamental configurations. For this it is not necessary to know the effective Hamiltonians $\mathcal{H}^{(i)}_{\text{eff}}$ explicitly.

We will not discuss the different methods for the computation of critical properties from the generated spin configurations on the *multigrid* $\Lambda^{(0)} \cup \Lambda^{(1)} \cup \cdots \cup \Lambda^{(n)}$ in detail. Important examples are:

Wilson's *matching method* for the determination of critical couplings [34]: For most models the critical coupling is not known exactly. The *matching method* is based on the fact that a renormalization group fixed point can only exist if the theory is exactly at criticality. The method has the advantage that by starting the blocking procedure from lattices with different size *finite size effects* can be reduced systematically.

The *matching method* for the determination of the $\Delta\beta$-function [37]: In the neighbourhood of a fixed point which has only one instable direction a scale transformation can be compensated by tuning a single parameter of the Hamiltonian (e.g. the inverse temperature β). This defines a $\Delta\beta$-function that can be determined by *matching* of correlation functions. Finite size effects can be reduced systematically by choosing fundamental lattices of different size.

A well known method is *Swendsen's procedure* for the computation of critical exponents [36]: The linearized renormalization group in the neighbourhood of a fixed point can be considered as an ∞-dimensional matrix T acting in the space of effective coupling constants. The components of this matrix can be expressed in terms of (connected) correlation functions of the block spins $\phi^{(i)}$ and $\phi^{(i+1)}$ and thus can be computed by Monte Carlo. The critical exponents of a theory are determined by the eigenvalues of T. The method has produced impressive results. However, errors coming from a necessary truncation of the ∞-dimensional matrix T are hard to estimate. The procedure takes advantage of the fact that the critical slowing down of certain observables which build up the matrix T is partially cancelled.

There is a large number of MCRG methods for the computation of effective Hamiltonians[1], but nearly all of them are based on Monte Carlo simulations of the full theory. Exceptions are a method due to Petronzio and Callaway [39], Gupta's IMCRG (Improved Monte Carlo Renormalization Group) [40] and more recent work which deals with the computation of the effective potential (free energy as a function of magnetization) for φ^4 theory [41].

[1] In a conference talk R. Gupta mentions 11 methods for the computation of effective couplings (October 1986) [40].

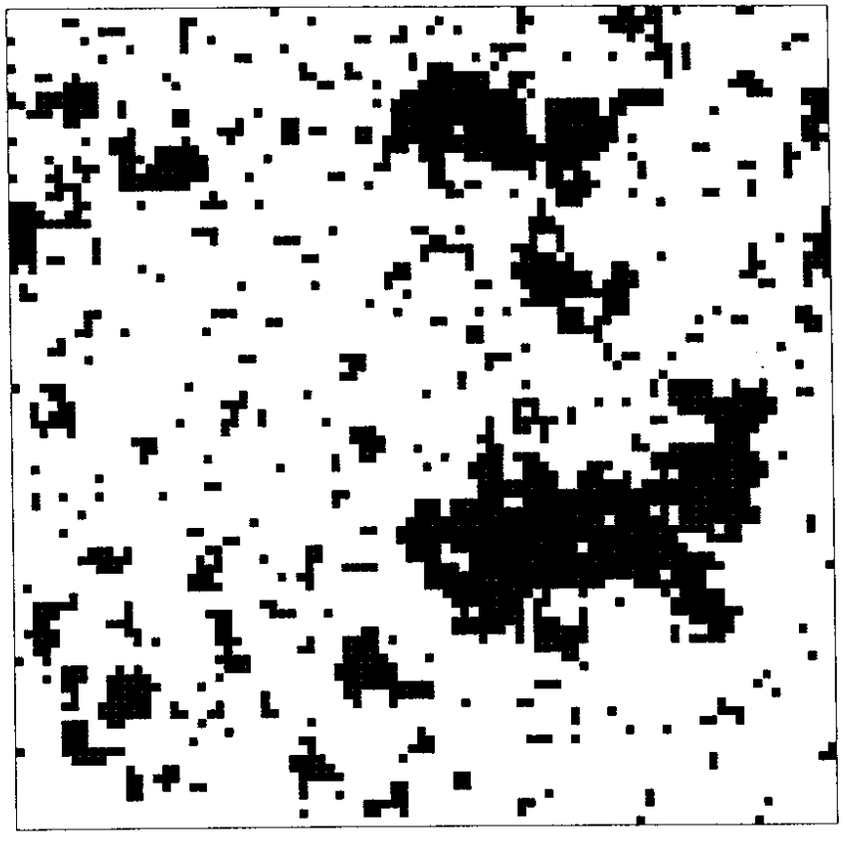

Figure I.2. A typical configuration of the 2-dimensional Ising model at the critical point. The black squares represent spins with $s = +1$. The corresponding white areas are crowded by spins with negative sign. The picture gives an impression of the scenario that is typical for a continuous phase transition: Because of the infinite correlation length no length scale is dominating, and fluctuations over all length scales occur. As a consequence there is no typical size of domains (areas of spins with equal sign). The renormalization group is a tool for a systematic and quantitative investigation of such systems. The fluctuations are integrated out scale by scale, and each integration step (= block spin transformation) is determined by an auxiliary statistical mechanical system with small correlation length. The scale invariance of the theory at large distances allows an approximate determination of the critical properties of the system after a *finite* number of block spin transformations.

Chapter II

Computation of Effective Hamiltonians for the O(N) Symmetric Nonlinear σ-Model by "Integration over β"

The derivative of the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ with respect to β is the expectation value of the fundamental Hamiltonian in the auxiliary statistical mechanical system with partition function $\exp\{-\mathcal{H}_{\text{eff}}(\phi)\}$ (= "auxiliary system with fixed block spins").

Monte Carlo simulations of the auxiliary system allow to compute $(\partial/\partial\beta)\mathcal{H}_{\text{eff}}(\phi)$. The effective Hamiltonian is then determined by integration over β. The initial value $\mathcal{H}_{\text{eff}}(\phi)|_{\beta=0}$ can either be computed exactly or be approximated very precisely with the help of the Central Limit Theorem of classical statistical mechanics [28].

Following Wilson's renormalization group philosophy one expects that correlations in the auxiliary system are of short range, at least in the small field region.[1] Monte Carlo simulations with fixed block spins therefore should not suffer from critical slowing down and large finite size effects.

The method described in this chapter requires Monte Carlo simulations for many different block spin configurations and β-values (cf. Wilson's remark cited in the Introduction). However, it will be shown that the procedure is well suited to compute the effective potential $\mathcal{V}_{\text{eff}}(\phi)$ (= effective Hamiltonian per volume for constant block spin).

Details of the Monte Carlo procedure are worked out for the O(N) symmetric nonlinear σ-model. In contrast to MCRG studies for this model in the literature [36,37], we will use linear block spin transformations that lead to block spins of fluctuating length. The Monte Carlo algorithm for the generation of spin configurations with fixed block spins is based on a simultaneous updating of randomly selected pairs of spins belonging to the same block.

Results of Monte Carlo calculations are presented for the Ising model and for the O(3) model on 2-dimensional lattices.

The 2-dimensional Ising model is exactly soluble [20]. It has a continuous (second order) phase transition at $\beta_c = \frac{1}{2}\ln(\sqrt{2}+1) = 0.440687$ which separates the symmetric phase from the phase with spontaneously broken symmetry. At the critical point the correlation length diverges and one expects the existence of a renormalization group fixed point.

By Monte Carlo simulations with constant background fields ϕ I computed the effective potential of the 2-dimensional Ising model for block size $L \leq 16$ and for $\beta \leq 0.6$. Thus the renormalization group flow of the potential can be studied in the symmetric and in the broken phase. At the Curie point one finds a renormalization group fixed point with critical exponents which are consistent with the exactly known values $\eta = 0.25$ and $\nu = 1.0$.

[1] Analytical renormalization group studies for weakly coupled theories [18] show that inside large field islands long range correlations might occur, cf. the discussion of the large field problem in Chapter III.1.

For a comparison with the Monte Carlo data I performed an $O(\beta^2)$ high temperature expansion for the effective potential of the 2-dimensional Ising model (Appendix A.1.). This expansion is surprisingly good. Qualitatively the renormalization group flow in the high temperature approximation behaves correctly. There even exists an (approximate) fixed point at $\beta = 0.9\,\beta_c$.

At the transition from the symmetric to the broken phase the simulation of the auxiliary system with fixed block spins is hampered by critical slowing down, especially when $\phi \approx 0$. Possibly this is not only a large field problem but might also have to do with the discontinuous phase transition of the Ising model in the broken phase [45].

The 2-dimensional O(N) model for $N \geq 3$ is renormalizable in perturbation theory and asymptotically free [23]. It is therefore expected that a continuum limit exists when the lattice spacing $a \to 0$ and $\beta \to \infty$ in a manner dictated by perturbation theory. In addition it is expected that the correlation length remains finite for all $\beta < \infty$. Thus for finite β a nontrivial fixed point should not exist. One expects that the effective potential will have an absolute minimum at $\phi = 0$ if the cutoff is low enough.

I computed the effective potential for the O(3) model for block size $L \leq 16$ and for $\beta \leq 2$ by Monte Carlo simulations with fixed constant block spins. Even at large β no critical slowing down shows up in the simulations with fixed block spins. This is remarkable, since the correlation length of the O(3) model at $\beta = 2$ exceeds $\xi = 100$ [26]. In the investigated range of β and block size the renormalization group flow meets the expectation: With decreasing cutoff the effective potential becomes more and more flat and evolves towards a convex shape.

By Monte Carlo simulations of the auxiliary system with $\beta = 0$ I determined coefficients of an $O(\beta^2)$ high temperature expansion for the effective potential of the O(3) model (Appendix A.2.). A comparison with the Monte Carlo data shows (for small enough blocks) an impressive quality of this expansion up to very large β-values where the correlation length can be larger than $\xi = 100$.

For large β one can expect that the renormalization group scenario is consistent with perturbative scaling. By a matching procedure for the effective potential a nonperturbative $\Delta\beta$-function is defined which can be compared with perturbation theory. It is found that in the range $\beta = 1.6 \ldots 2.0$ the scaling behaviour of the effective potential comes close to the perturbative prediction.

This chapter is organized as follows:

II.1. Block Spins of Fluctuating Length for the O(N) Model

Linear block spin transformations are defined for the O(N) symmetric nonlinear σ-model on the lattice. Notion and meaning of the effective potential are explained.

The partition function of the O(N) symmetric nonlinear σ-model is

$$Z \equiv \int \prod_{z \in \Lambda} ds(z)\, e^{-\beta \mathcal{H}(s)} \equiv \int \mathcal{D}s\, e^{-\beta \mathcal{H}(s)} \tag{1-1}$$

We will use lattice units, i.e. lattice spacing $\equiv 1$. Finite lattices shall be provided with periodic boundary conditions. The dimensionless spins $s(z)$ are integrated over with the uniform measure on the $(N-1)$-dimensional unit sphere S^{N-1}, $ds = d^N s \cdot \delta(s^2 - 1)$.

$\beta \geq 0$ is the inverse temperature. We consider ferromagnetic spin models with nearest neighbour interaction and Hamiltonian

$$\mathcal{H}(s) = -\sum_{<v,w>} s(v) \cdot s(w) \tag{1-2}$$

The sum $\sum_{<v,w>}$ runs over all (unordered) pairs of nearest neighbour sites (= links).

For $N = 1$ the δ-function can be integrated out exactly, and one arrives at the partition function of the Ising model:

$$Z_{\text{Ising}} = \Big(\prod_{z \in \Lambda} \sum_{s(z) = \pm 1}\Big)\, e^{-\beta \mathcal{H}(s)} \equiv \sum_{s} e^{-\beta \mathcal{H}(s)} \tag{1-3}$$

We now define renormalization group transformations for the O(N) model. Dimensionless block spin variables $\phi(x)$, $x \in \Lambda'$, are defined by

$$\phi(x) = \lambda \operatorname*{av}_{z \in x} s(z) \tag{1-4}$$

with $\lambda = L^{\frac{1}{2}(d-2)}$. A wave function can be taken into account later by a suitable rescaling of the block spin field. ($\lambda = L^{\frac{1}{2}(d-2+\eta)}$ in the neighbourhood of a renormalization group fixed point, cf. Chapter I.)

ϕ is a block spin of fluctuating length, with $0 \leq |\phi(x)| \leq \lambda$. For $N \geq 2$ the block spins can vary continuously within this sphere. The Ising model has discrete block spin values: $L^d \phi(x) = \lambda[-L^d, -L^d + 2, \ldots, L^d - 2, L^d]$.

An effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ is defined by

$$e^{-\mathcal{H}_{\text{eff}}(\phi)} = \int \mathcal{D}s\, e^{-\beta \mathcal{H}(s)} \prod_{x \in \Lambda'} \delta[\phi(x) - \lambda \operatorname*{av}_{z \in x} s(z)] \equiv \mathcal{Z}(\phi) \tag{1-5}$$

(In the Ising case the δ-function is considered as a Kronecker-δ.) Integrating $\mathcal{Z}(\phi)$ over the block spin variables the partition function is recovered:

$$\int \prod_{x\in\Lambda'} d^N\phi(x)\, \mathcal{Z}(\phi) = Z \tag{1-6}$$

$d^N\phi$ denotes the Lebesgue measure on R^N. In the Ising case one has to sum over the discrete values of the block spins:

$$\sum_{\phi} \mathcal{Z}_{\text{Ising}}(\phi) = Z_{\text{Ising}} \tag{1-7}$$

It is easy to see that the effective theory inherits the invariance of the fundamental model under global O(N) transformations. Let $\hat{O} \in O(N)$. Then

$$\begin{aligned} e^{-\mathcal{H}_{\text{eff}}(\hat{O}\phi)} &= \int \mathcal{D}s\, e^{-\beta\mathcal{H}(s)} \prod_{x\in\Lambda'} \delta[\hat{O}\phi(x) - \lambda \operatorname*{av}_{z\in x} s(z)] \\ &= \int \mathcal{D}s\, e^{-\beta\mathcal{H}(s)} \prod_{x\in\Lambda'} \delta[\phi(x) - \lambda \operatorname*{av}_{z\in x} \hat{O}^{-1}s(z)] \\ &= \int \mathcal{D}s\, e^{-\beta\mathcal{H}(\hat{O}s)} \prod_{x\in\Lambda'} \delta[\phi(x) - \lambda \operatorname*{av}_{z\in x} s(z)] \\ &= e^{-\mathcal{H}_{\text{eff}}(\phi)} \end{aligned} \tag{1-8}$$

The restriction of the block spins to compact (or discrete) subsets of R^N implies singularities of $\mathcal{H}_{\text{eff}}(\phi)$ at the boundaries of the domain of ϕ. The effective Boltzmannian $\mathcal{Z}(\phi)$ vanishes if $|\phi(x)| \geq \lambda$ for some $x \in \Lambda'$. At these points the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ diverges to infinity.

The effective potential[1] $\mathcal{V}_{\text{eff}}(\phi)$ is defined as effective Hamiltonian per volume for constant block spin field ϕ:

$$\mathcal{V}_{\text{eff}}(\phi) \equiv \mathcal{H}_{\text{eff}}(\phi)\big|_{\varphi=\text{const}}/|\Lambda'| \tag{1-9}$$

($|\Lambda'|$ denotes the number of block lattice sites.) The motivation for this notion is the following: $\mathcal{D}\phi \exp[-|\Lambda'|\mathcal{V}_{\text{eff}}(\phi)]$ is the probability distribution of the block spins ϕ in the subspace of constant configurations. If the block lattice consists of a single site, $\mathcal{V}_{\text{eff}}(\phi)$ is free energy as a function of β and magnetization. The shape of $\mathcal{V}_{\text{eff}}(\phi)$ for a ferromagnet will depend on β and on the block size. The correlation length of the fundamental spins can (very roughly) be considered as the typical extension of areas in the lattice where spins are strongly aligned. If these regions are considerably larger than the lattice spacing of the effective theory under consideration, then the effective potential will have minima at $|\phi| \neq 0$. If the correlation length is finite by lowering the UV-cutoff (via block spin transformations) it can be achieved that the correlation length in units of the block lattice spacing is of order one. The effective potential then should have a unique minimum at $\phi = 0$. (In the O(3) model the transition of the potential from a mexican hat shape to a single well shape takes place

[1] $\mathcal{V}_{\text{eff}}(\phi)$ depends only on $|\phi|$.

when the correlation length is about half of the block size L, cf. Figure II.5.4.). More precise than these considerations is the following statement: If for low enough cutoff the effective Hamiltonian can be written in the form

$$\begin{aligned} \mathcal{H}_{\text{eff}}(\phi) = &\quad \text{kinetic term} \quad + \quad \sum_x \mathcal{V}_{\text{eff}}[\phi(x)] \\ &+ \quad \text{small nonlocal terms involving } \nabla\phi \end{aligned} \tag{1-10}$$

and if the effective potential has a unique minimum at $\phi = 0$, then the fundamental theory has finite correlation length.[1] This follows from a semiclassical analysis [9]. Brydges, Fröhlich and Spencer prove the existence of a mass gap under the assumption that the small nonlocal correction terms can be neglected or considered as small perturbations [14].

II.2. A Method to Compute $\mathcal{H}_{\text{eff}}(\phi)$ by Monte Carlo

The derivatives of the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ with respect to β are truncated moments of the fundamental Hamiltonian in the auxiliary statistical mechanical system with partition function $\exp[-\mathcal{H}_{\text{eff}}(\phi)]$. Monte Carlo simulations of this system therefore allow to compute especially $(\partial/\partial\beta)\mathcal{H}_{\text{eff}}(\phi)$ for arbitrary block spin configurations ϕ.

The Monte Carlo method is a method to compute expectation values. However, the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ is logarithm of a partition function (see Eq. (1-5)):

$$\mathcal{H}_{\text{eff}}(\phi) = -\ln \mathcal{Z}(\phi) \tag{2-1}$$

But note that

$$\frac{\partial}{\partial\beta}\mathcal{H}_{\text{eff}}(\phi) = -\mathcal{Z}(\phi)^{-1}\frac{\partial}{\partial\beta}\mathcal{Z}(\phi) = \langle\mathcal{H}(s)\rangle_{\phi,\beta} \tag{2-2}$$

The ϕ-parametric expectation $\langle(\cdot)\rangle_{\phi,\beta}$ is defined by

$$\langle\mathcal{O}(s)\rangle_{\phi,\beta} \equiv \mathcal{Z}(\phi)^{-1} \int \mathcal{D}s\, e^{-\beta\mathcal{H}(s)} \prod_{x\in\Lambda'} \delta[\phi(x) - \lambda \operatorname*{av}_{z\in x} s(z)]\, \mathcal{O}(s) \tag{2-3}$$

One might also consider higher derivatives: For $n \geq 1$

$$\left(\frac{\partial}{\partial\beta}\right)^n \mathcal{H}_{\text{eff}}(\phi) = (-1)^{n+1}\langle\mathcal{H}^n(s)\rangle^T_{\phi,\beta} \tag{2-4}$$

$\langle(\cdot)\rangle^T$ denotes the truncated expectation value[2].

[1] "Kinetic term" here means a term quadratic in ϕ which vanishes for constant ϕ.

[2] $\ln\langle e^x\rangle \equiv \sum_{n\geq 1} \frac{\langle x^n\rangle^T}{n!}$; $\langle x\rangle^T = \langle x\rangle$; $\langle x^2\rangle^T = \langle x^2\rangle - \langle x\rangle^2$ etc.

Expectation values $\langle(\cdot)\rangle_{\phi,\beta}$ can be computed using the Monte Carlo method. Details of the procedure will be described in Section II.3.

The differential equation $\frac{\partial}{\partial\beta}\mathcal{H}_{\text{eff}}(\phi) = \langle\mathcal{H}(s)\rangle_{\phi,\beta}$ can be solved by integration over β:

$$\mathcal{H}_{\text{eff}}(\phi) = \mathcal{H}_{\text{eff}}(\phi)|_{\beta=0} + \int_0^\beta d\beta' \langle\mathcal{H}(s)\rangle_{\phi,\beta'} \tag{2-5}$$

The computation of the initial value $\mathcal{H}_{\text{eff}}(\phi)|_{\beta=0}$ is trivial for the Ising model (Appendix A.1.). For $N \geq 3$ very precise approximations have been worked out, based on the Central Limit Theorem of classical statistical mechanics [28].

In order to compute $\mathcal{H}_{\text{eff}}(\phi)$ one needs to know $\langle\mathcal{H}(s)\rangle_{\phi,\beta'}$ for $\beta' < \beta$. However, it will suffice to do Monte Carlo simulations for a relatively small number of β-values. The intermediate values then can be obtained by interpolation, for example with splines. For small enough β no Monte Carlo simulations need to be done since high temperature expansions can be used.

A disadvantage of the described method is that already the computation of $\mathcal{H}_{\text{eff}}(\phi)$ for a single configuration ϕ requires some effort. This is acceptable if one can assume that $\mathcal{H}_{\text{eff}}(\phi)$ is of a simple form with few parameters. However, in general the effective Hamiltonian is a functional which depends on ϕ in a complicated way. If one cannot assume a simple form for $\mathcal{H}_{\text{eff}}(\phi)$, then a careful study requires Monte Carlo simulations for many of block spin configurations. This is inconvenient. However, the situation is better for the effective potential. $\mathcal{V}_{\text{eff}}(\phi)$ depends only on a single real or discrete variable (Ising model). In later chapters we will study Taylor expansions of the effective Hamiltonian in the block spin variables, with Taylor coefficients obtained by differentiating $\ln\mathcal{Z}(\phi)$ with respect to the $\phi(x)$. This is easy to do in the case of a Gaussian block spin transformation (Chapter III) or for φ^4 theory with δ-block spin (Chapter IV). For the O(N) model with δ-block spin derivatives with respect to the $\phi(x)$ are not so easy to perform. The Ising model has discrete block spins, and naive differentiation is impossible. For $N \geq 2$ Taylor expansions in the block spin fields should exist, but the constraints $s(z)^2 = 1$ make it difficult to remove the ϕ-dependence from the non-analytical δ-function.

II.3. Monte Carlo Simulations with Fixed Block Spins

A Monte Carlo algorithm is described which updates spin configurations while holding block spins fixed. The procedure is based on a simultaneous update of randomly selected pairs of spins belonging to the same block. The algorithm cannot be applied in the case N=2.[1]

We first discuss the generation of initial configurations. This is done blockwise in such a way that the start configuration of the spins in block x only depends on $\phi(x)$.

Generation of a start configuration for the Ising model:
We want to generate an s-configuration of the spins in block x which obeys the condition

[1] The 2-dimensional O(2) model (*planar rotator* or *XY-model*, [22]) will not be discussed in this paper. Possibly in the block spin definition for this model in addition to block averages *winding numbers* have to be taken into account in order to represent topological excitations (*vortices*) of the model properly.

$$\sum_{z\in x} s(z) = L^d\lambda^{-1}\phi(x) \tag{3-1}$$

Of course, ϕ has to be given such that this is possible. One first computes

$$N_+(x) = \text{number of spins in } x \text{ with } s(z) = +1 \;=\; \frac{L^d}{2}[1 + \lambda^{-1}\phi(x)] \tag{3-2}$$

Then all sites $z \in x$ are visited, in arbitrary order. The first $N_+(x)$ spin variables are set to $+1$, the other spins are set to -1. For $\beta \neq 0$ the resulting configuration will not be a typical one, i.e. it will be a configuration that is unlikely to occur in a sequence of configurations distributed according to the measure defined by Eq. (2-3). Concrete Monte Carlo simulations (see Sections II.4. and II.5.) were always started with $\beta = 0$, and then the system was successively "cooled" down. This is natural because in order to perform the integration over β one needs measurements for a sequence of β-values starting from $\beta = 0$. For $\beta = 0$ all configurations with the prescribed block averages have the same probability, and any initial configuration is as good as another one.

Generation of a start configuration for the O(N) model:
Without restriction of generality one can assume that $\phi(x)$ points in N-direction. (If this is not the case it can be achieved by some suitably chosen rotation $\hat{O} \in O(N)$. After initializing the spins in x the inverse matrix $\hat{O}^{-1}$ is applied to each spin separately.) Let $\phi(x) = |\phi(x)| \cdot \hat{e}_N$. ($\hat{e}_N$ denotes the unit vector in N-direction in spin space.) First one sets $s_N(z) \equiv \lambda^{-1}\phi(x)$ for all $z \in x$. The other spin components now have to be adjusted in such a way that

$$\begin{aligned} &\sum_{i=1}^{N-1} s_i(z)^2 = 1 - s_N(z)^2 \\ &\sum_{z\in x} s_i(z) = 0 \quad \text{for} \quad i = 1,\ldots,N-1 \end{aligned} \tag{3-3}$$

We discuss the case that the block volume L^d is even. Then the spins can be considered pair by pair. We consider a pair of spins $s(z_1)$ and $s(z_2)$. The vector of the first $N-1$ components of s will be called $\hat{s}$. $\hat{s}(z_1)$ is a vector of length $[1 - s_N(z_1)^2]^{\frac{1}{2}}$. One generates a random vector with this property. Then one defines $\hat{s}(z_2) \equiv -\hat{s}(z_1)$. Repeating this for all spin pairs, one obtains an "allowed" (and for $\beta = 0$ also "generic") spin configuration.

Monte Carlo updating for Ising configurations:
The probability distribution for Ising configurations s with fixed block spins ϕ is given by

$$\text{prob}(s) \propto e^{-\beta\mathcal{H}(s)} \prod_{x\in\Lambda'} \delta[\phi(x) - \lambda \operatorname*{av}_{z\in x} s(z)] \tag{3-4}$$

In an updating sweep single spins cannot be "flipped" without violating the restriction that the block averages of the spins must not be changed. The elementary excitation of the system is an exchange of positions: Two spins in the same block which have different sign exchange their sites. By successive exchanges of sites any configuration with the prescribed block

average can be reached. We consider pairs of spins $\{s_1, s_2\} \equiv \{s(z_1), s(z_2)\}$ with $z_1 \in x$ and $z_2 \in x$. Under the condition that all the other spins are kept fixed, the probability distribution for the possible orientations of the two spins is given by

$$\text{prob}(s_1, s_2) \propto e^{\beta(t_1 s_1 + t_2 s_2 + \epsilon s_1 s_2)} \delta[s_1 + s_2 - s_{12}] \tag{3-5}$$

Here we have defined:

$$\begin{aligned} \epsilon &\equiv \begin{cases} 1 & \text{if} \quad z_1, z_2 \quad \text{nearest neighbours} \\ 0 & \text{else} \end{cases} \\ t_1 &\equiv \sum_{<z_1, z>} s(z) - \epsilon\, s_2 \\ t_2 &\equiv \sum_{<z_2, z>} s(z) - \epsilon\, s_1 \end{aligned} \tag{3-6}$$

s_{12} is the sum of the spins before the updating: $s_{12} \equiv s_1^{\text{old}} + s_2^{\text{old}}$. In the case $s_{12} \neq 0$ the spins s_1 and s_2 must not be changed. Thus one can assume that $s_2 = -s_1$, and one finds

$$\text{prob}(s_1)\big|_{s_2 = -s_1} \propto e^{\beta(t_1 - t_2) s_1} \tag{3-7}$$

The ϵ-term has been absorbed by the normalization constant. The probability distribution is easily normalized:

$$\text{prob}(s_1 = 1)\big|_{s_2 = -s_1} = [1 + e^{-2\beta(t_1 - t_2)}]^{-1} \tag{3-8}$$

$t_1 - t_2$ is an integer between $-4d$ and $+4d$. Thus the possible values of $\text{prob}(s_1 = 1)$ can be computed before the Monte Carlo run. This avoids a frequent call of the exponential function. An elementary updating is done as follows: Given a pair of spins s_1 and s_2 belonging to the same block, $s_1 \neq s_2$, one reads $\text{prob}(s_1 = 1)$ from a table. Then a uniform random number is taken from the interval $0 < rnd < 1$. If $rnd < \text{prob}(s_1)$, set $s_1 = 1$ and $s_2 = -1$. Else the other way round, i.e. $s_1 = -1$ and $s_2 = +1$.

Monte Carlo updating for $O(N \geq 3)$ configurations:
As in the case of the Ising model one considers the conditional probability distribution for a pair of spins $\{s_1, s_2\}$ belonging to the same block x.

$$\text{dprob}(s_1, s_2) \propto d^N s_1 d^N s_2\, \delta[s_1^2 - 1]\, \delta[s_2^2 - 1]\, \delta[s_1 + s_2 - s_{12}]\, e^{\beta(t_1 s_1 + t_2 s_2 + \epsilon s_1 s_2)} \tag{3-9}$$

The definitions of ϵ, t_i, s_{12} are the same as above. We perform the following nonsingular transformation of variables:

$$\begin{aligned} s_+ &= s_1 + s_2 \\ s_- &= s_1 - s_2 \end{aligned} \tag{3-10}$$

The value of s_+ must not be changed: $s_- \equiv s_{12} = s_1^{\text{old}} + s_2^{\text{old}}$. The conditional probability distribution for s_- is given by

$$\text{dprob}(s_-) \propto d^N s_-\, \delta[s_+^2 + s_-^2 + 2 s_+ s_- - 4]\, \delta[s_+^2 + s_-^2 - 2 s_+ s_- - 4]\, e^{\beta[\frac{1}{2}(t_1 - t_2) s_- - \frac{1}{4}\epsilon s_-^2]} \tag{3-11}$$

The product of the two δ-functions can be written in a more suggestive form:

$$\delta[s_+^2 + s_-^2 + 2 s_+ s_- - 4]\, \delta[s_+^2 + s_-^2 - 2 s_+ s_- - 4] \propto \delta[s_+^2 + s_-^2 - 4]\, \delta[s_+ s_-] \tag{3-12}$$

The proof of this formula is simple if one uses the Fourier representation of the δ-function:

$$\begin{aligned} &\delta[s_+^2 + s_-^2 + 2 s_+ s_- - 4]\, \delta[s_+^2 + s_-^2 - 2 s_+ s_- - 4] \\ &\propto \int dq_1 dq_2\, e^{iq_1[s_+^2 + s_-^2 + 2 s_+ s_- - 4]}\, e^{iq_2[s_+^2 + s_-^2 - 2 s_+ s_- - 4]} \\ &\propto \int dq_1 dq_2\, e^{i(q_1 + q_2)[s_+^2 + s_-^2 - 4]}\, e^{i(q_1 - q_2)[2 s_+ s_-]} \\ &\propto \int dq_+ dq_-\, e^{iq_+[s_+^2 + s_-^2 - 4]}\, e^{iq_-[2 s_+ s_-]} \\ &\propto \delta[s_+^2 + s_-^2 - 4]\, \delta[s_+ s_-] \end{aligned} \tag{3-13}$$

One thus obtains

$$\text{dprob}(s_-) \propto d^N s_-\, \delta[s_-^2 - (4 - s_+^2)]\, \delta[s_+ s_-]\, e^{\frac{1}{2}\beta(t_1 - t_2) s_-} \tag{3-14}$$

At this point it is easy to see that for O(2) configurations pairwise updating is not sufficient.[1] For 2-dimensional vectors s_- the equation $s_+ s_- = 0$ has only two solutions, which differ only in sign. Thus the only possible change would be a change in the sign of s_-. This is equivalent to exchanging sites of s_1 and s_2. With the exception of the Ising case such an algorithm cannot be ergodic.

To generate vectors s_- which are distributed according to $\text{dprob}(s_-)$ one can employ the *Metropolis* algorithm [29]. A transition $s_-^{\text{old}} \to s_-^{\text{new}}$ is proposed which obeys the restrictions of the two δ-functions. The exponential factor is then taken into account by a "Metropolis filter". s_- is restricted to the (N-2)-dimensional sphere of vectors with length $[4 - s_+^2]^{\frac{1}{2}}$ which are perpendicular to s_+. There are two special cases which however occur with "zero probability": $s_+^2 = 4$ (s_1 and s_2 are parallel). Then $s_- = 0$, and nothing is to be done; $s_+^2 = 0$ (s_1 and s_2 are antiparallel), then $s_-^2 = 4$, and the direction of s_- is arbitrary. In the context of a computer simulation one will forgo an updating if either $4 - s_+^2 < \kappa$ or $s_+^2 < \kappa$, for example with $\kappa = 10^{-6}$.

[1] For the updating of O(2) configurations with fixed block averages one needs a procedure which updates at least three spins simultaneously.

We will denote the sphere of vectors with length r perpendicular to s_+ by $S^\perp(s_+,r)$. An algorithm will now be described which generates random vectors s_- which are uniformly distributed on $S^\perp(s_+,r)$: At first one generates a random vector v which with equal probability lies anywhere in the unit ball $B^N \equiv \{v \in R^N : v^2 < 1\}$. (A sequence of such vectors can be obtained by dropping from a sequence of vectors uniformly distributed in the cube $-1 < v_i < 1$ all vectors whose length exceeds 1.) In a second step v is projected onto the subspace perpendicular to s_+ and subsequently rescaled to length r. This can be done with the help of the map $\mathcal{P}$:

$$\mathcal{P}: \quad B^N \to \quad S^\perp(s_+,r), \quad v \to \mathcal{P}v = r \cdot \frac{s_+^2 v - (vs_+)s_+}{|s_+^2 v - (vs_+)s_+|} \tag{3-15}$$

If $N = 3$ one can use a more simple procedure: A random vector with uniform distribution on the "circle" $S^\perp$ can be obtained by a rotation of s_-^{old} about the axis s_+ with a randomly chosen angle $0 \le \alpha < 2\pi$:

$$s_-^{\text{old}} \to s_-^{\text{new}} = (\cos\alpha)\, s_-^{\text{old}} + (\sin\alpha)\,[\frac{s_+}{|s_+|} \times s_-^{\text{old}}] \tag{3-16}$$

"$\times$" denotes the vector product of vectors in R^3. A complete updating for the spin pair $\{s_1, s_2\}$ is performed as follows. Given $\{s_1, s_2\}$, one determines s_+. If $4 - s_+^2 < \kappa$ or $s_+^2 < \kappa$ no update is performed. Else one first determines s_-^{old} and $t_1 - t_2$. Now $\mathcal{N}$ Metropolis hits are applied which consist of the following steps: 1. Generate a candidate s_-^{new} with uniform probability distribution on $S^\perp(s_+,(4-s_+^2)^{\frac{1}{2}})$, as described above. 2. Generate a random number $0 < rnd < 1$. s_-^{new} is accepted as the new value of s_- if

$$\omega \equiv e^{\frac{1}{2}\beta(t_1-t_2)[s_-^{\text{new}} - s_-^{\text{old}}]} \ge rnd \tag{3-17}$$

Otherwise one sets $s_-^{\text{new}} \equiv s_-^{\text{old}}$.

Organization of a complete sweep through the lattice:
One sweeps through the block lattice Λ', systematically or in a random way. At block x one considers successively all sites $z_1 \in x$. Given z_1, with uniform probability one of the sites $z_2 \in x - z_1$ is selected as updating partner.[1] If the blocks are not too small it is possible to exclude nearest neighbour pairs from updating. This does not violate the condition of detailed balance and has two advantages: The computation of $t_1 - t_2$ is considerably simplified. The second advantage can be explained most easily for the Ising model. Because of the ferromagnetic interaction neighbouring spins are most likely to be aligned. In this case updating is not possible. Therefore an algorithm which updates nearest neighbour pairs will be less effective compared to an updating algorithm for more distant spins.

[1] A *vectorization* of the algorithm is only possible if the random partner selection is dropped. When choosing fixed partner relations one has to make sure that the algorithm is ergodic.

II.4. The Effective Potential for the 2-Dimensional Ising Model
Monte Carlo Results

Monte Carlo results for the effective potential of the 2-dimensional Ising model are presented. Data have been taken for block size $L \le 16$ and for $\beta \le 0.6$.

Parameters of the Monte Carlo experiment:
56 Monte Carlo runs were done for each of the block sizes $L = 4$, $L = 8$ and $L = 16$. For constant block spin fields $\phi = \{\frac{0}{8}, \frac{1}{8}, ..., \frac{7}{8}\}$ and for $\beta = \{0.0, 0.1, ..., 0.6\}$ always 100×100 heat bath updating sweeps (as described in Section II.3.) were performed. After each sweep the observable "energy per block" was measured. The data from 100 successive sweeps were averaged during the Monte Carlo run. So for each configuration of parameters (L, ϕ, β) we have 100 data points. The following table displays lattice parameters and the consumed computer time on the scalar computer [*49*].

blocks	block lattice	CPU/h
4×4	15×15	10.6
8×8	10×10	18.8
16×16	6×6	27.2

The mean CPU needed for the update of a single spin pair was approximately 19 μsec.

critical slowing down?
Following Wilson's renormalization group philosophy one expects that there are no critical fluctuations in the auxiliary system with fixed block spins, even if the fundamental theory has large or infinite correlation length. Thus a Monte Carlo simulation of the auxiliary system should not suffer from critical slowing down. One expects a fast equilibration of the system and only small sweep to sweep correlations. But certain circumstances might lead to long range correlations in the auxiliary system:

1. The block size L is too large. One cannot expect that lowering the cutoff over many scales at once is a manageable problem. The idea of the renormalization group is to integrate over the fluctuations in small manageable steps. In a Monte Carlo procedure designed in this spirit one would perform only a single renormalization group step at a time, with small block size L. However, in order to iterate renormalization group transformations such a procedure would require knowledge of a sufficiently precise approximation of $\mathcal{H}_{\text{eff}}(\phi)$ after each step, for example in terms of coupling constants. This is not easy to achieve. Another way to fight critical slowing down is to use *multigrid* methods [*31*]: Several scales are integrated over at once but one introduces separate variables (block spins) for each length scale involved in the problem. In constrast to a pure renormalization group procedure the probability distributions for the block spins are computed again and again. This looks at first sight uneconomical but it avoids the hard problem to determine approximate (truncated) effective Hamiltonians which, used in Monte Carlo simulations, will reproduce the long distance behaviour of the theory correctly.

2. The background field ϕ contains huge large field islands.[1] In analytical renormalization group studies [18] for a given block spin configuration ϕ the block lattice Λ' is divided into large field region and small field region. The small field region consists of the block lattice sites where the effective Hamiltonian is (locally) small. The large field region is the complement of the small field region. For weakly coupled theories it turnes out that for a generic block spin configuration nearly all sites of the block lattice are in the small field region, and big large field islands have small probability. In the small field region $\mathcal{H}_{\text{eff}}(\phi)$ has good locality properties and the auxiliary system with fixed block spin ϕ shows only short range correlations. However, within the large field islands one has to be aware of long range correlations, the effective Hamiltonian becomes very large (locally) and has bad locality properties. Fields in the large field region are not necessarily large by value. For a ferromagnet with a pronounced local minimum of the effective potential at $\phi \neq 0$ sites x with $\phi(x) \approx 0$ can be in the large field region.

3. The system is close to a first order phase transition. There is evidence [45] that renormalization group transformations might become singular in the neighbourhood of discontinuous phase transitions. This might be relevant for the Ising model at $\beta > \beta_c$, because in this model for $\beta > \beta_c$ there is a first order phase transition for external magnetic field $= 0$. The strength of this transition increases when β becomes larger. It is an interesting question whether this problem vanishes at the critical point.

[1] The *large field problem* will be discussed in some detail in Chapter III.1.

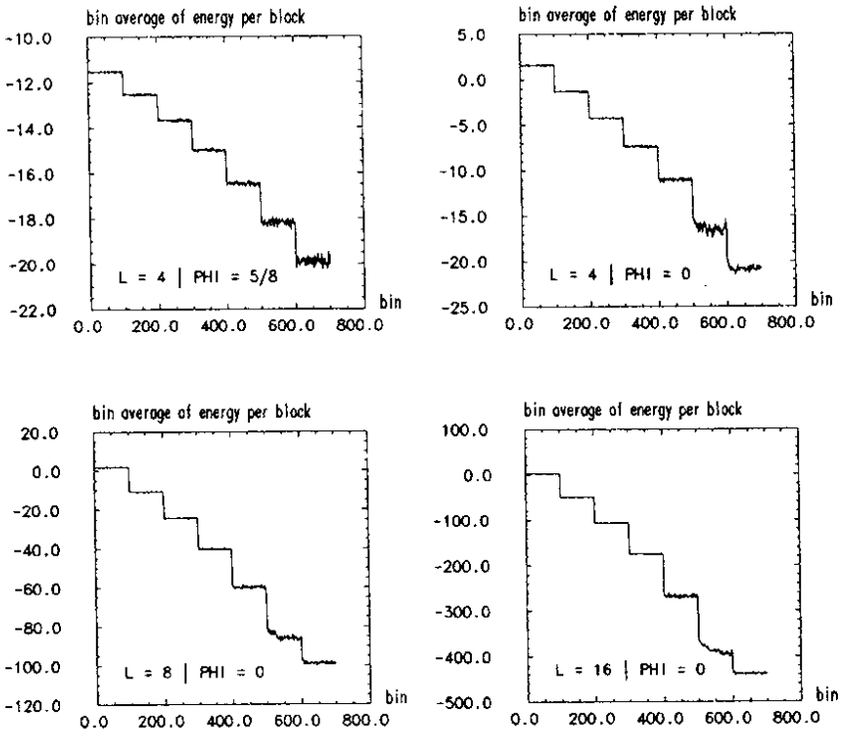

Figure II.4.1. "Time evolution" of the bin averages of $\mathcal{H}(s)$ per block with fixed constant block spin ϕ. The Monte Carlo simulations for a given value of the background field were started with $\beta = 0$. Always after 10^4 sweeps ($= 100$ bins with 100 sweeps) β was increased by 0.1. The steps in the diagrams, looked at from the left to the right, thus correspond to β-values $0.0/0.1/.../0.6$. For $L = 4$ and $\phi = \frac{5}{8}$ equilibration is very fast, even below the Curie point at $\beta = 0.440687$. Significant critical slowing down is observed for $\phi = 0$ and larger block size L. Possibly it is not only a large field problem but is also due to the neighbourhood of the line of first order phase transitions in the broken phase of the Ising model [45].

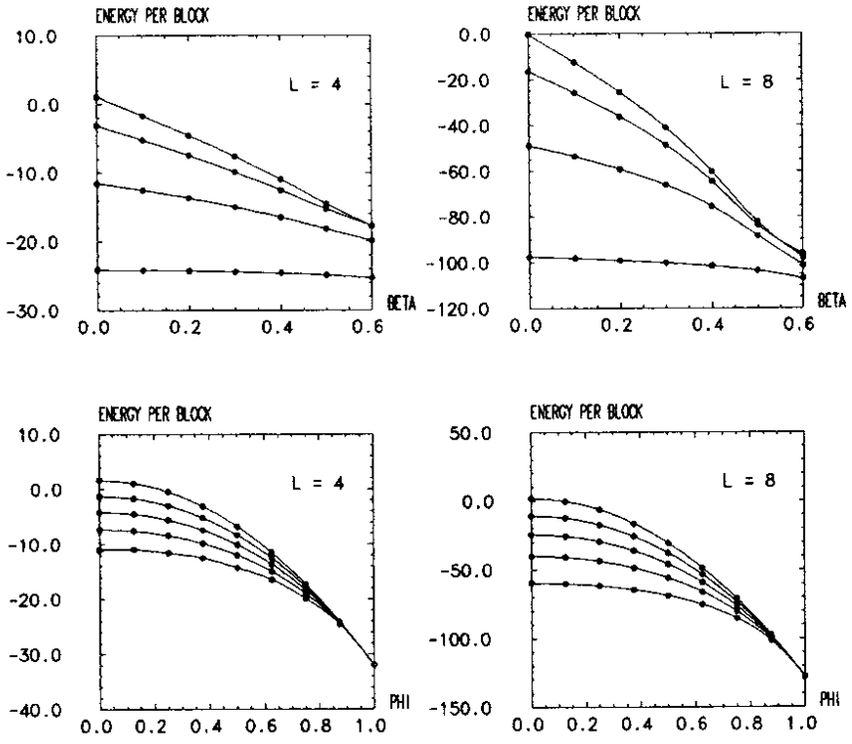

Figure II.4.2. Monte Carlo results for the expectation values $\langle \mathcal{H}(s) \rangle_{\phi,\beta} / |\Lambda'|$ for $L = 4$ and $L = 8$. The averages are given as functions of β and as functions of the constant block spin ϕ. The Monte Carlo results are plotted as small circles, with statistical errors smaller than the diameters of the circles.

Top: the curves correspond to ϕ-values $\{\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}\}$, read from top to bottom. The full lines are spline interpolations. By integration of these splines over β one computes the effective potential $\mathcal{V}_{\text{eff}}(\phi)$ (see figures on the next pages).

Bottom: the β-values (from top to bottom) are 0.0/0.1/0.2/0.3/0.4. The spline interpolation curves allow a continuation of the data to ϕ-values for which no Monte Carlo simulations have been performed.

For this plot ϕ was not rescaled, i.e. $\lambda \equiv 1$.

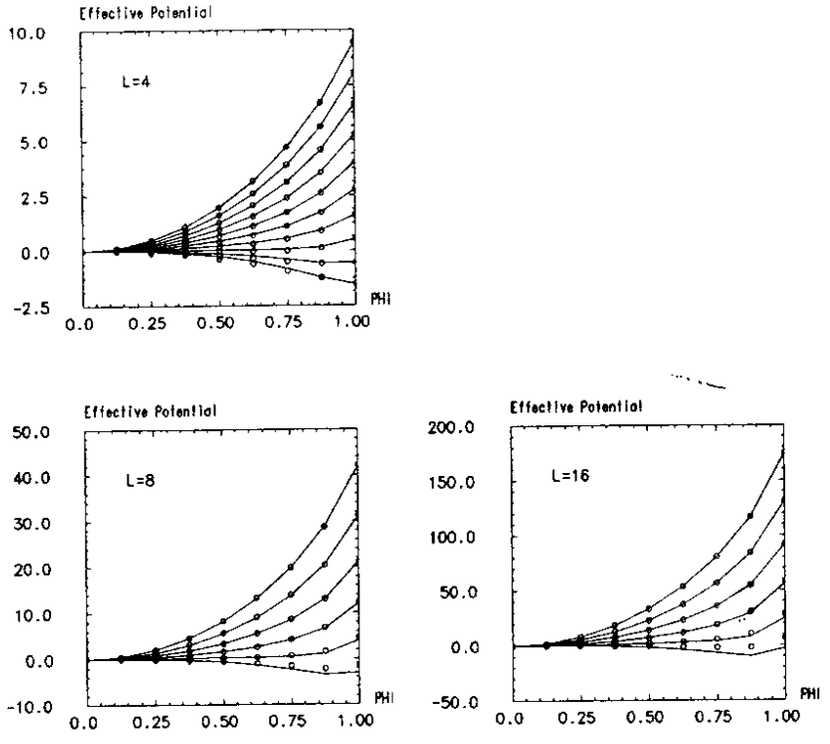

Figure II.4.3. Monte Carlo results for the effective potential $\mathcal{V}_{\text{eff}}(\phi)$ of the 2-dimensional Ising model and comparison with high temperature expansions. The full lines are interpolation curves for the Monte Carlo results. The circles show results of an $O(\beta^2)$ expansion for $\mathcal{V}_{\text{eff}}(\phi)$ (see Appendix A.1.).

For block size $L = 4$ the curves, from top to bottom, correspond to $\beta/\beta_c = 0.0/0.1/.../0.9$.

For $L = 8$ and $L = 16$ the results are displayed for $\beta/\beta_c = 0.0/0.2/.../1.0$.

For this figure ϕ was not rescaled, i.e. $\lambda \equiv 1$.

For small blocks the high temperature expansion is surprisingly good. See also Figure II.4.8.

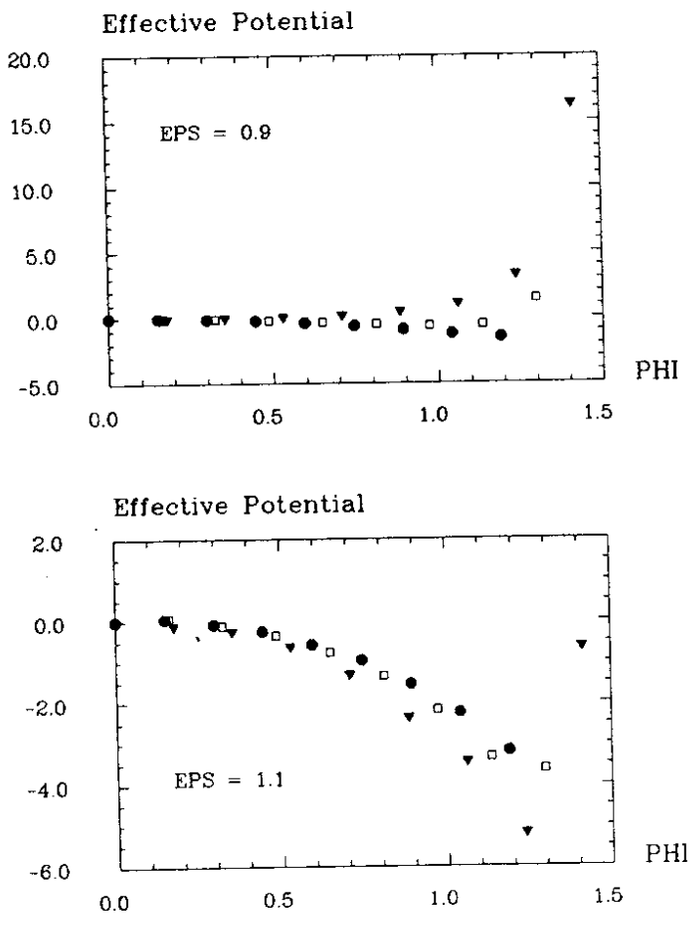

Figure II.4.4. The renormalization group flow in the symmetric ($\beta/\beta_c \equiv \epsilon = 0.9$) and in the broken phase ($\epsilon = 1.1$). The different symbols belong to different block size: dots ($L = 4$), squares ($L = 8$) and triangles ($L = 16$). For $\epsilon = 0.9$ the effective potential with decreasing cutoff acquires a convex shape. For $L = 16$ the minimum is already at $\phi = 0$. In the phase with spontaneously broken symmetry a minimum at $|\phi| \neq 0$ grows deeper and deeper.

For this figure ϕ was rescaled according to $\eta = 0.25$, i.e. $\lambda \doteq L^{\frac{1}{4}}$.

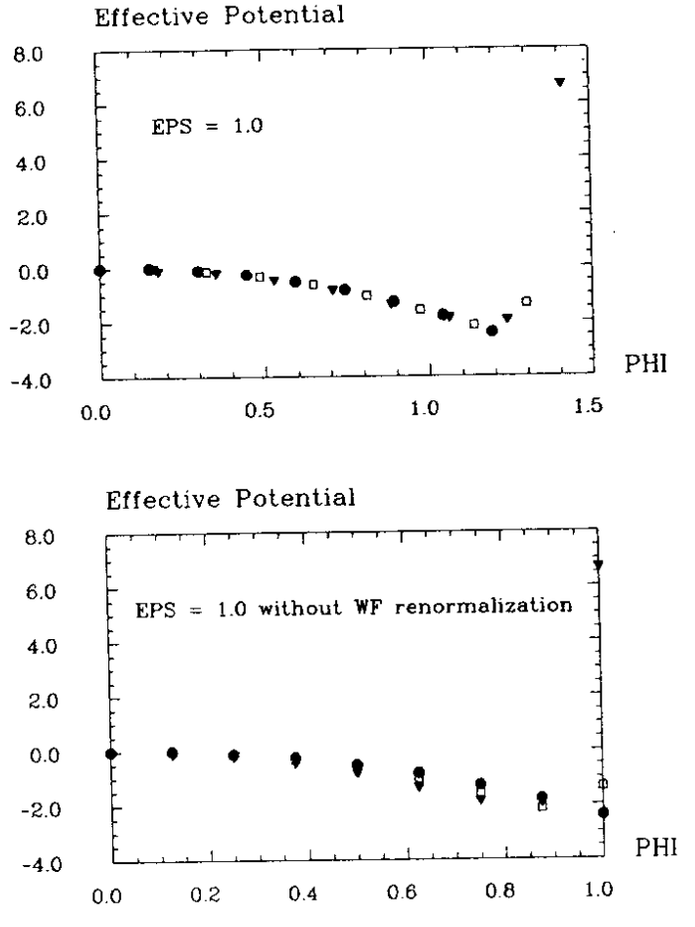

Figure II.4.5. Renormalization group flow of the effective potential on the critical surface. The upper picture shows the fixed point potential. The meaning of the symbols is the same as in Figure II.4.4. The second picture clearly shows that without a wave function renormalization no fixed point behaviour can be observed.

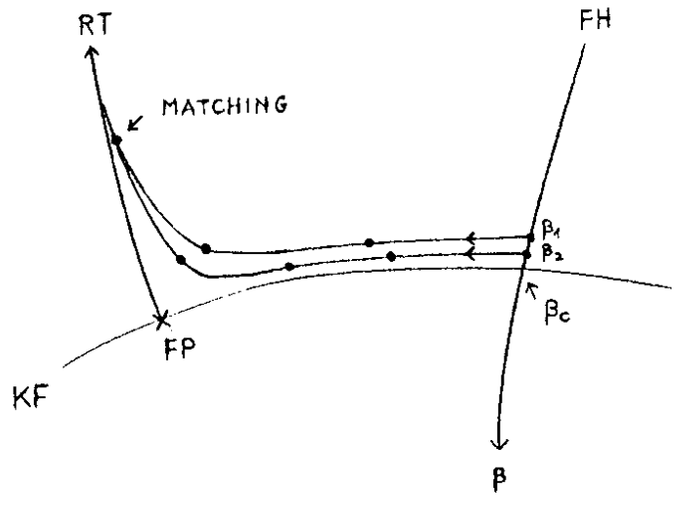

Figure II.4.6. The renormalization group scenario for the Ising model in the symmetric phase. The picture shows a projection of the ∞-dimensional space of effective Hamiltonians onto the 2-dimensional drawing plane.

KF is the critical surface. On this surface there are all the Hamiltonians which define theories with infinite correlation length ξ. The fundamental nearest neighbour Hamiltonians $\beta\mathcal{H}$, labeled by β, lie on FH. The line FH intersects the critical surface at $\beta = \beta_c$.

Under iterated renormalization group transformations the critical Hamiltonian $\beta_c\mathcal{H}$ converges to the fixed point FP. All Hamiltonians attracted by FP belong to the same universality class, i.e. have the same critical exponents.

Fundamental Hamiltonians with $\beta < \beta_c$ approach the 1-dimensional renormalized trajectory RT.

We consider renormalization group transformations with a scale factor L. Let $\mathcal{R}^k\{\beta\mathcal{H}\}$ be the effective Hamiltonian obtained by k successive block spin transformations (or a single one with a scale factor L^k) from $\beta\mathcal{H}$. If $\mathcal{R}^k\{\beta_1\mathcal{H}\} \approx \mathcal{R}^{k+1}\{\beta_2\mathcal{H}\}$ for $\beta_1 < \beta_2$ (*matching* along RT), then the correlation lengths of the fundamental model at β_1 and β_2 differ by a factor of L. This is so because

$$\xi[\mathcal{R}^k\{\beta_1\mathcal{H}\}] = \xi[\mathcal{R}^{k+1}\{\beta_2\mathcal{H}\}],$$

$$\frac{\xi(\beta_1)}{L^k} = \frac{\xi(\beta_2)}{L^{k+1}} \tag{4-1}$$

$$\xi(\beta_2) = L \cdot \xi(\beta_1)$$

For temperatures $T \equiv \beta^{-1}$ close above the Curie temperature T_c

$$\xi(T) \propto (T - T_c)^{-\nu} \tag{4-2}$$

In terms of the variable $\epsilon \equiv \beta/\beta_c < 1$

$$\xi(\epsilon) \propto \left(\frac{1}{\epsilon} - 1\right)^{-\nu} \tag{4-3}$$

For ϵ_1 and ϵ_2 sufficiently close to 1 it follows from Eq. (4-1) that

$$\frac{\xi(\epsilon_2)}{\xi(\epsilon_1)} = L = \frac{(\frac{1}{\epsilon_2} - 1)^{-\nu}}{(\frac{1}{\epsilon_1} - 1)^{-\nu}} \tag{4-4}$$

$$\ln L = \nu \cdot \ln\left\{\frac{\epsilon_2}{\epsilon_1} \cdot \frac{(1-\epsilon_1)}{(1-\epsilon_2)}\right\}$$

The following table shows pairs ϵ_1, ϵ_2 obtained from a *matching* procedure for the effective potentials with $L = 8$ and $L = 16$ (see Figure II.4.7.). The resulting values for the exponent ν are close to the exact value $\nu = 1$ [2].

ϵ_1	ϵ_2	ν
0.950	0.975	0.96
0.960	0.980	0.97
0.970	0.985	0.98
0.980	0.990	0.99

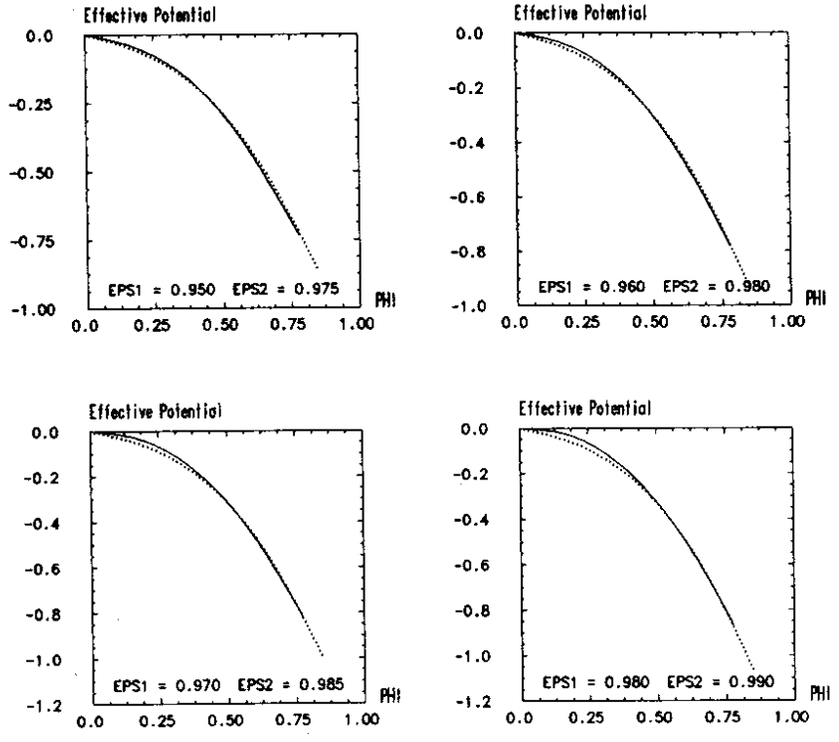

Figure II.4.7. *Matching* along the renormalization group trajectory. The pictures show splines for the effective potential, rescaled according to $\eta = 0.25$. The section with $\phi > 0.8$ is suppressed since no matching can be expected there.[1] The full curves belong to $L = 8$ and $\beta/\beta_c = \epsilon_1$. The dotted lines show the potential for block size $L = 16$ and $\beta/\beta_c = \epsilon_2$. For given ϵ_1 the coupling ϵ_2 was determined such that the matching of the two curves in a region around $\phi \approx 0.5$ was best. The procedure is sensitive to inaccuracies. However, it shows consistency of the Monte Carlo results with the exactly known value $\nu = 1$.

[1] The effective potential for block size L diverges at $\phi = L^{\frac{\beta}{\nu}} = L^{\frac{1}{8}}$. In the limit $L \to \infty$ this pole is shifted to infinity, and exact matching becomes possible.

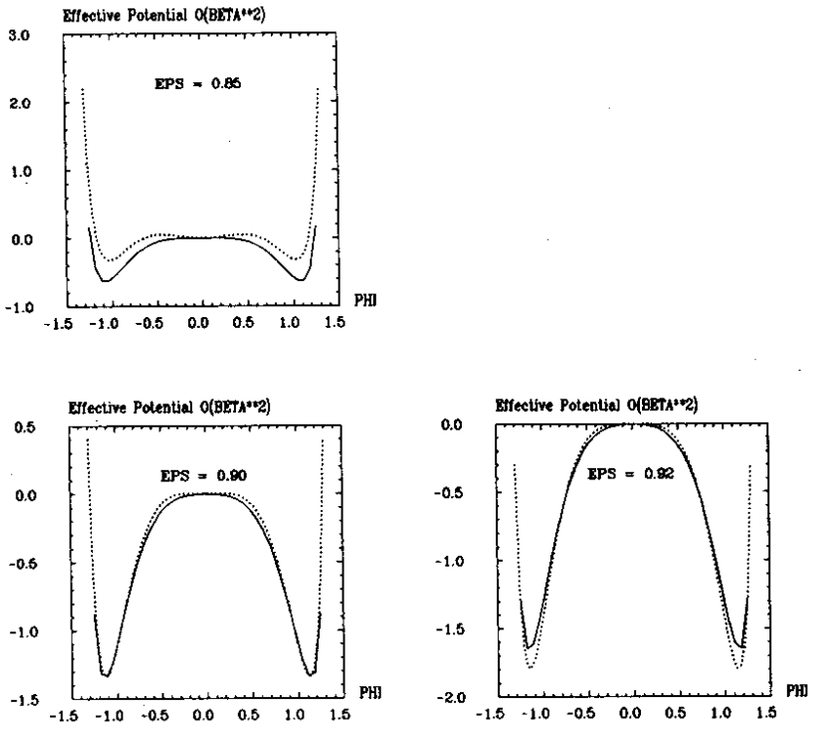

Figure II.4.8. Results of an $O(\beta^2)$ high temperature expansion for the effective potential of the 2-dimensional Ising model. The pictures show the effective potential in the $O(\beta^2)$ approximation (see Appendix A.1.), rescaled according to $\eta = 0.25$. The potentials for block size $L = 6$ are plotted with full lines, dotted lines belong to block size $L = 8$. Qualitatively the renormalization group flow is reproduced correctly. There is an (approximate) fixed point at $\beta/\beta_c \equiv \epsilon = 0.9$. For $\beta < 0.9$ the potential is driven to a single well shape, whereas for $\beta > 0.9$ the behaviour in the phase with spontaneously broken symmetry imitated.

II.5. The Effective Potential for the 2-Dimensional O(3) Model Monte Carlo Results

Monte Carlo results for the effective potential of the 2-dimensional O(3) model are presented. Data have been collected for block size $L \leq 16$ and for $\beta \leq 2$.

Parameters of the Monte Carlo experiment:
77 Monte Carlo runs were done for each of the block sizes $L = 4$, $L = 8$ and $L = 16$: For each value of the constant background field $\phi = \{0.0, 0.15, ..., 0.9\}$ and for $\beta = \{0.0, 0.2, ..., 2.0\}$ always 100×50 updating sweeps (as described in Section II.3.) were performed. The elementary update of the spin pairs was done using a 2-hit Metropolis algorithm. For all β-values the acceptance rate was better than 50%. After each sweep the observable "energy per block" was measured. The averages of the observable over 50 successive sweeps were determined during the Monte Carlo simulation. Thus for each configuration of the parameters (L, ϕ, β) we have 100 data points. The following table displays lattice parameters and CPU time consumed on the scalar computer [*49*].

blocks	block lattice	CPU/h
4×4	10×10	10
8×8	8×8	33
16×16	5×5	54

The mean CPU needed for the updating of a single spin pair (two Metropolis hits) was about 70 μsec. This is 3.5 times slower than a heat bath update for the Ising model.

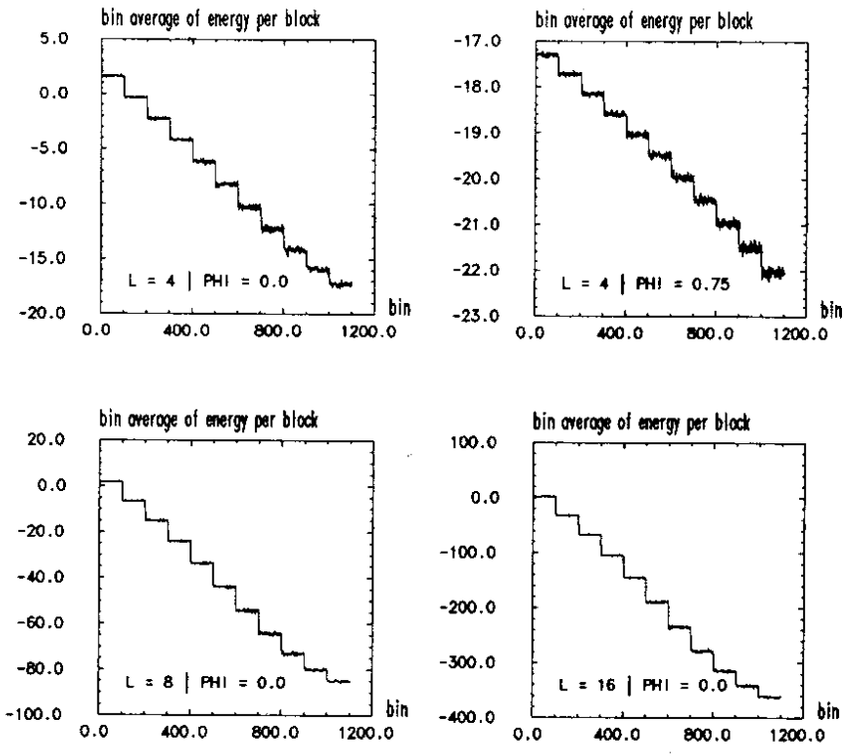

Figure II.5.1. "Time evolution" of the bin average of $\mathcal{H}(s)$ per block with fixed constant block spin ϕ. The Monte Carlo simulations for a given value of the background field were started with $\beta = 0$. Always after 5000 sweeps (= 100 bins with 50 sweeps) β was increased by 0.2. Thus the steps in the diagrams (from left to right) correspond to β-values 0.0/0.2/.../2.0. Even at large β equilibration is very fast, and there is no indication for critical slowing down.

For this figure we chose background field $\phi = 0$. For large β sites of the lattice where the block spin is close to $\phi = 0$ might belong to large field islands. Within such islands long range correlations can occur. Cf. the corresponding discussion for the Ising model, Figure II.4.1.

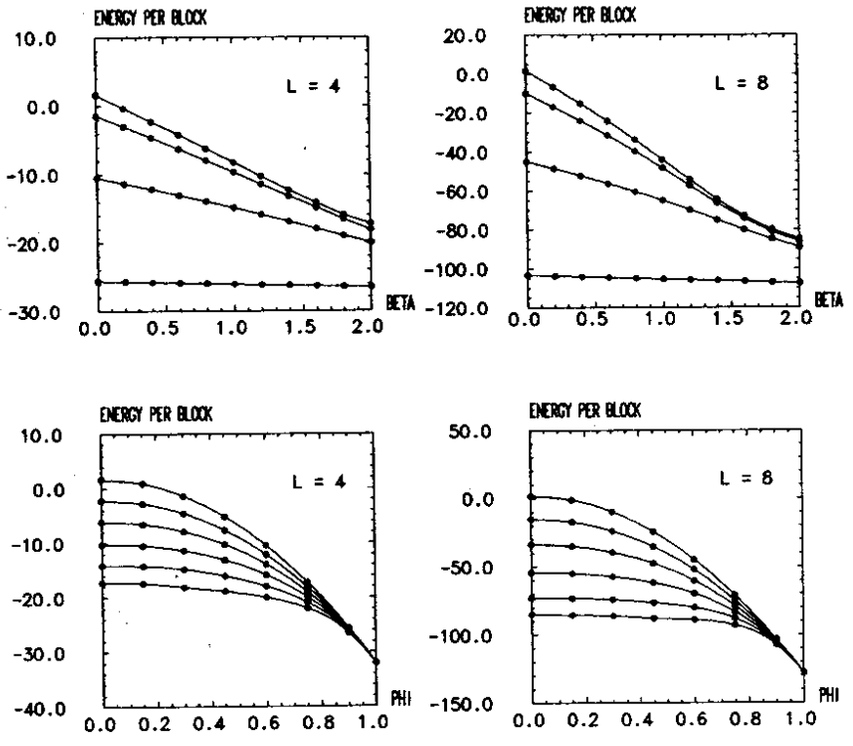

Figure II.5.2. Monte Carlo results for the expectation values $\langle \mathcal{H}(s) \rangle_{\phi,\beta}/|\Lambda'|$ for block size $L = 4$ and $L = 8$. The Monte Carlo averages are plotted as circles with statistical errors smaller than the diameters of the circles.

Top: from top to bottom the curves correspond to ϕ-values 0.0/0.3/0.6/0.9. The full lines are spline interpolation curves which allow a continuation of the Monte Carlo data to ϕ-values for which no simulations were done.

Bottom: from top to bottom the lines correspond to $\beta = 0.0/0.4/.../2.0$. The full lines are spline interpolation curves. Integration of these splines over β allows a computation of the effective potential $\mathcal{V}_{\text{eff}}(\phi)$.

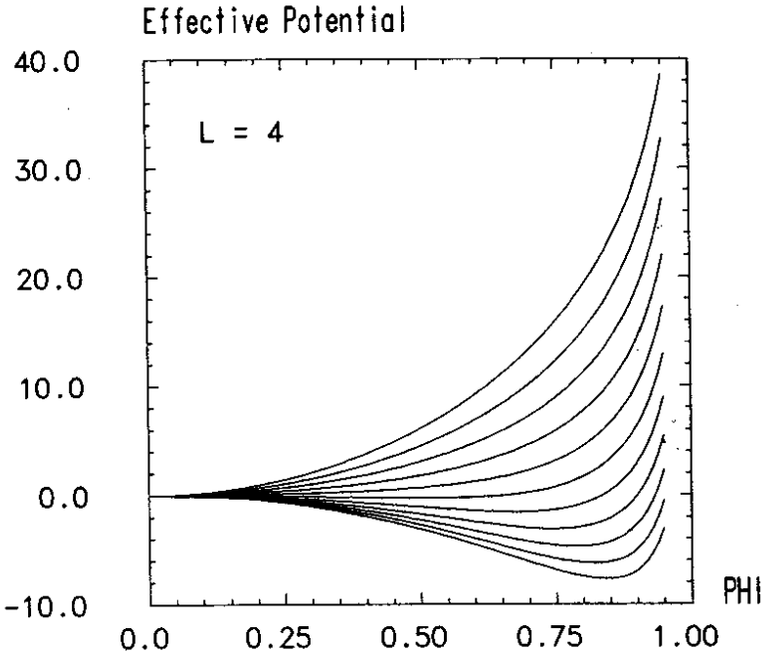

Figure II.5.3a. The effective potential for block size $L = 4$ and for $\beta \leq 2$.

From top to bottom the curves belong to β-values 0.0/0.2/.../2.0. The potentials were obtained by integration of the splines for $(\partial/\partial\beta)\mathcal{V}_{\text{eff}}(\phi) = \langle \mathcal{H}(s) \rangle_{\phi=\text{const}}/|\Lambda'|$. For the computation of $\mathcal{V}_{\text{eff}}(\phi)_{\beta=0}$ a FORTRAN-subroutine by P. Lützow [28] was used.

A constant was added to the potentials such that $\mathcal{V}_{\text{eff}}(0)$=0.

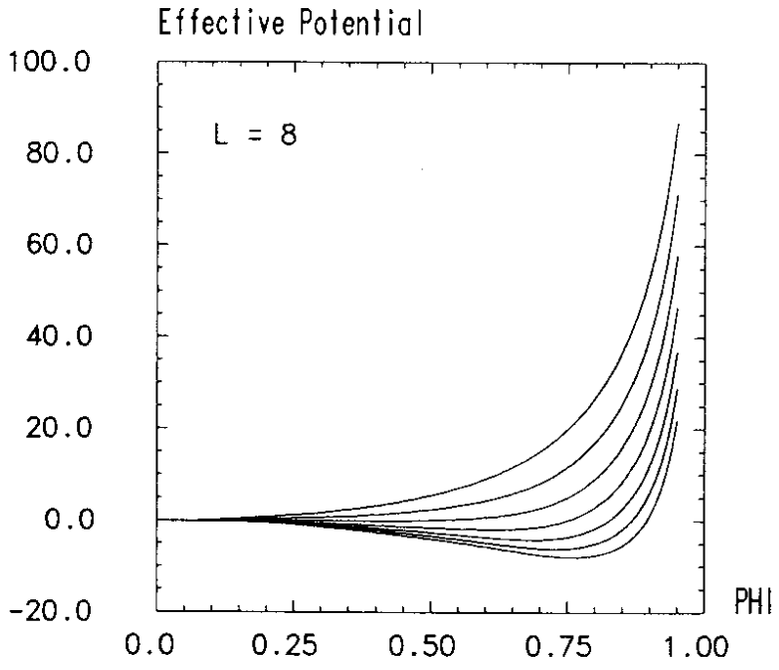

Figure II.5.3b. The effective potential for block size $L = 8$.

From top to bottom the curves correspond to β-values 0.8/1.0/.../2.0.

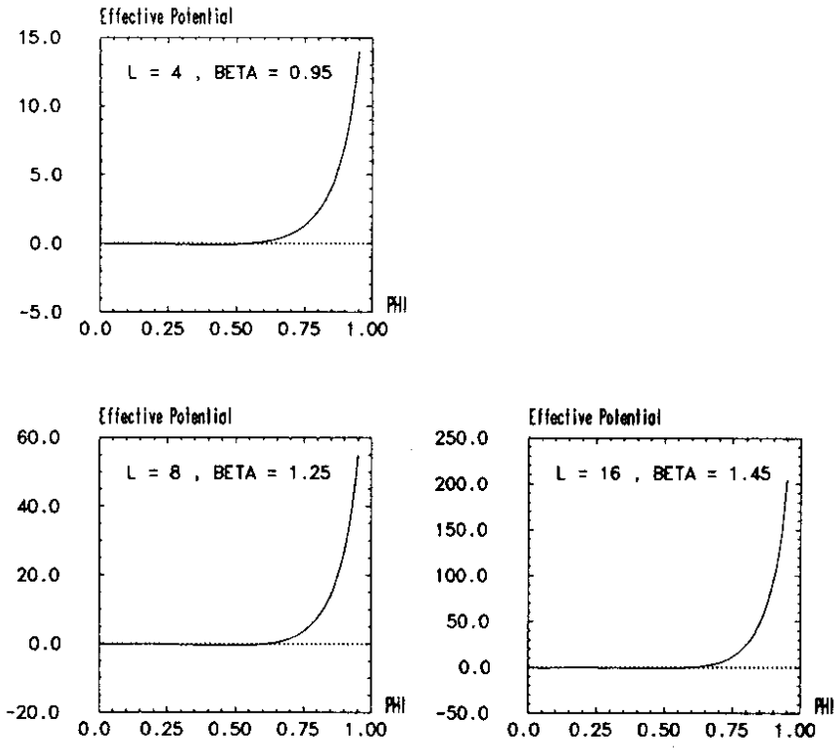

Figure II.5.4. Determination of the "transition point": For a given block size L there is a uniquely determined β-value $\tilde{\beta}(L)$ where the shape of the effective potential changes from "mexican hat" (local minima at $\phi \neq 0$) to "single well" (unique minimum at $\phi = 0$). A comparison with Monte Carlo results for the correlation length of the O(3) model shows that the "transition" occurs when the correlation length exceeds half of the block length L.

$$\xi(\beta = 0.95) \approx 1.7$$
$$\xi(\beta = 1.25) \approx 4.0$$
$$\xi(\beta = 1.45) \approx 9.0$$

This table is based on rough interpolation of Monte Carlo results taken from [*26*].

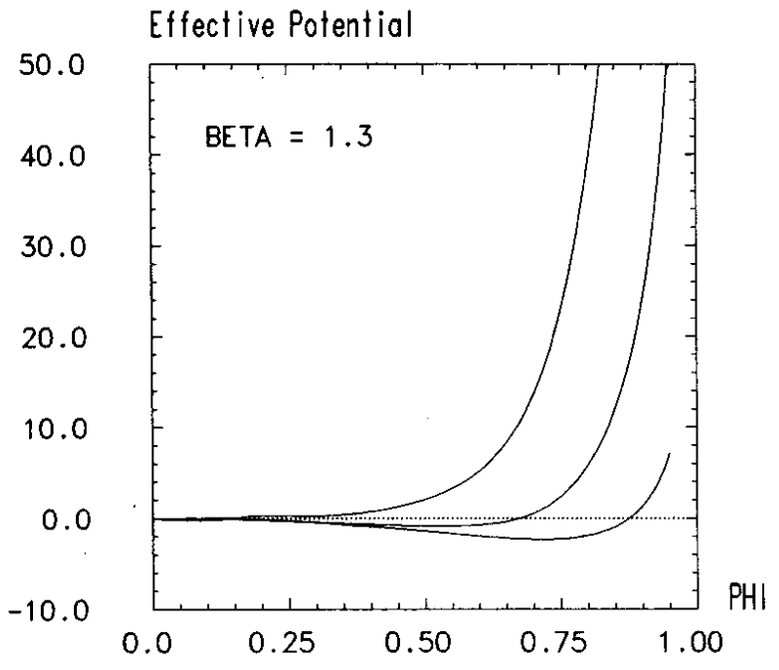

Figure II.5.5. The renormalization group flow of the effective potential with decreasing UV-cutoff. For $\beta = 1.3$ the potential was plotted for block size $L = 4$ (bottom), $L = 8$ (middle) and $L = 16$ (top). For $L = 16$ a convex shape has been reached.

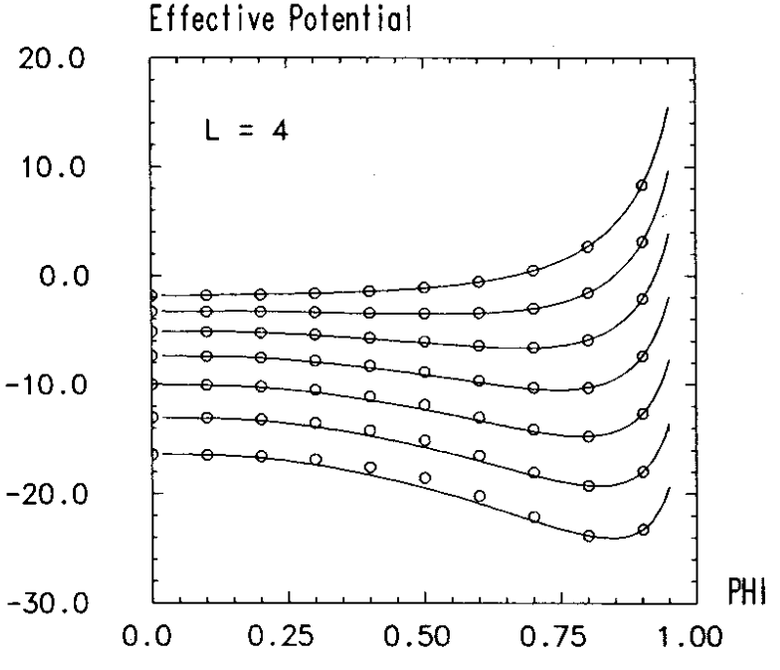

Figure II.5.6. Comparison of the effective potential for block size $L = 4$ with a Mayer expansion $O(\beta^2)$.

From top to bottom the curves belong to β-values 0.8/1.0/.../2.0.

The full lines are spline interpolation curves for the Monte Carlo data. The circles represent the results of an $O(\beta^2)$ expansion for the effective potential. The Mayer coefficients were obtained by Monte Carlo simulations of the auxiliary system at $\beta = 0$ (see Appendix A.3.). The quality of the high temperature approximation is remarkable: For $\beta \leq 1$ there are no deviations, and up to $\beta = 2$ depth and position of the minima are reproduced correctly.

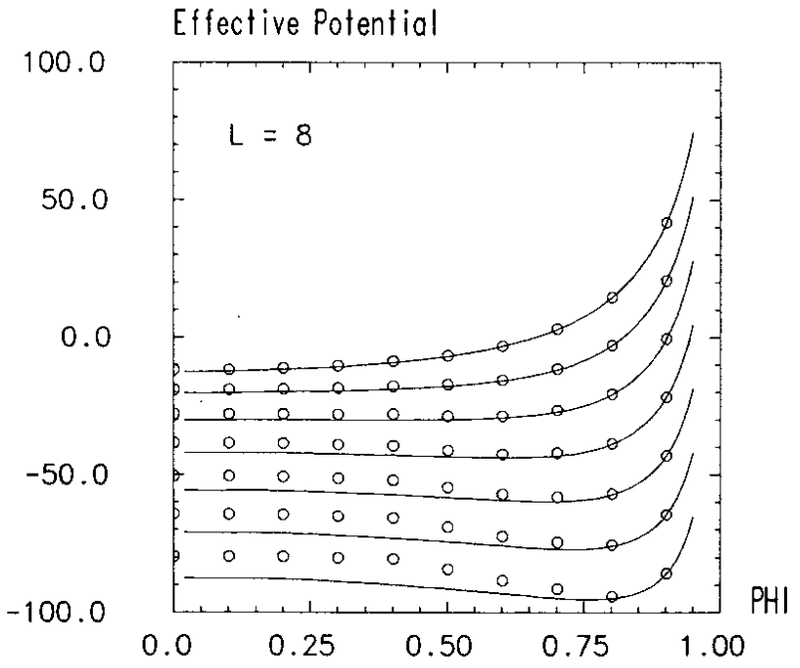

Figure II.5.7. Comparison of the effective potential for block size $L = 8$ with a Mayer expansion $O(\beta^2)$.

From top to bottom the curves belong to β-values 0.8/1.0/.../2.0.

Compared with block size $L = 4$ the quality of the high temperature approximation is worse. This problem might be tackled using iterated Mayer expansions [7,8]. These expansions are organized in such a way that only small scale factors L occur.

Asymptotic scaling?

2-loop perturbation theory predicts the following behaviour for the correlation length $\xi(\beta)$ of the $O(N \geq 3)$ model [27]:

$$\xi(\beta) = \text{const} \cdot \beta^{1/(2-N)} \cdot e^{2\pi\beta/(N-2)} \cdot \left[1 + O(\beta^{-1})\right] \tag{5-1}$$

Asymptotic scaling means that the perturbative correlation length sets the scale for all physical quantities. In particular one expects that theories with the same correlation length $\xi(\beta)$ have the same effective potential.

From the asymptotic formula for the correlation length one obtains the perturbative function $\Delta\beta_{per}$: Increasing the inverse temperature β by $\Delta\beta$ for large β is equivalent (up to a wave function renormalization) to a scale transformation with a scale factor of 2: $\xi(\beta + \Delta\beta) = 2 \cdot \xi(\beta)$. For N=3 one finds

$$\Delta\beta_{per} = \frac{\ln 2}{2\pi} \cdot \left[1 + \frac{1}{2\pi\beta}\right] + O(\beta^{-1}) \tag{5-2}$$

The following table shows the perturbative $\Delta\beta$ for several β-values compared to nonperturbative results from a matching procedure for the effective potential. $\Delta\beta_{23}$ was obtained from the renormalization group flow due to the transition from block size $L = 4$ to $L = 8$ (see Figure II.5.8.). The discrepancy to the perturbative predictions suggests the conclusion that after two or three $L = 2$ block spin transformation one is not close enough to the renormalized trajectory yet. $\Delta\beta_{34}$ was determined from a matching procedure for effective potentials belonging to block size $L = 8$ and $L = 16$ (see Figure II.5.9.). The agreement with the asymptotic $\Delta\beta$ is much better.

β	$\Delta\beta_{per}$	$\Delta\beta_{23}$	$\Delta\beta_{34}$
1.6	0.1213	0.06	0.10
1.7	0.1206	0.04	0.10
1.8	0.1201	0.03	0.08
∞	0.1032	-	-

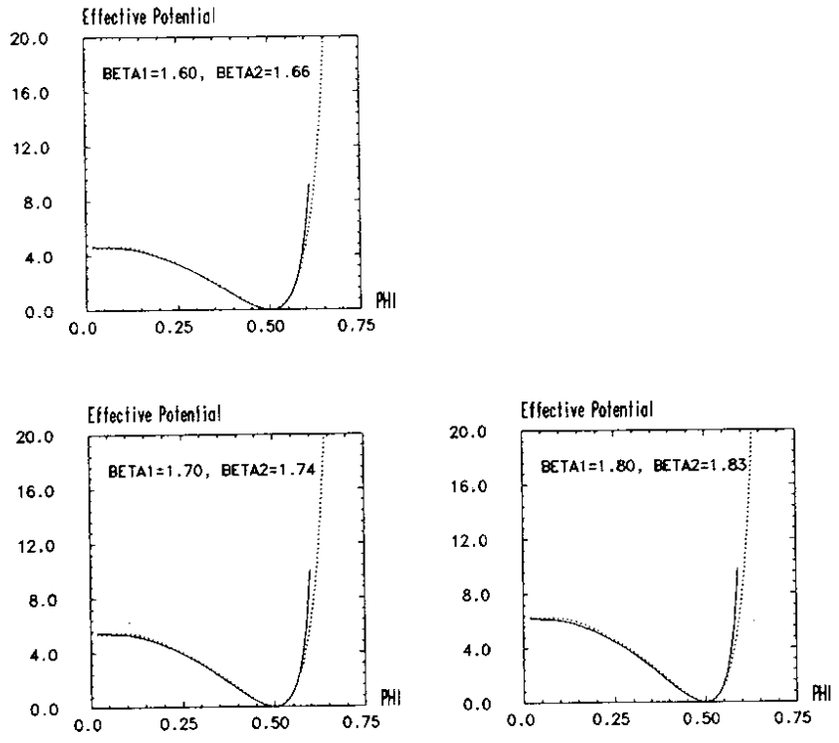

Figure II.5.8. Determination of $\Delta\beta$ with a matching procedure for the effective potential. The pictures show the effective potential for block size $L = 4$ (full lines) and $L = 8$ (dotted). The potentials have been rescaled such that their minimum is always at $\phi = 0.5$. (Without a condition of this kind no matching would be possible.) A constant was added such that $\mathcal{V}_{\text{eff}}(0.5) = 0$. $\beta = \beta_1$ was prescribed for $L = 4$. Then for block size $L = 8$ the coupling β_2 was determined such that the matching of the potentials (especially in the neighbourhood of the minimum) was best. The discrepancy of the $\Delta\beta$-values derived from this figure to the perturbative value $\Delta\beta_{per} \approx 0.12$ suggests that for block size $L = 4$ and $L = 8$ a universal renormalized trajectory has not yet been reached.

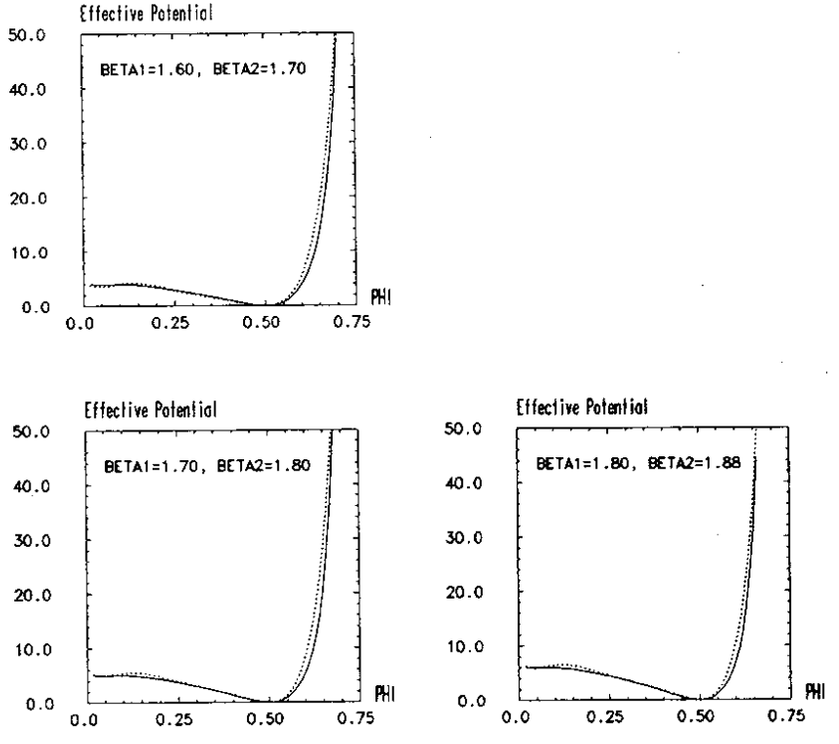

Figure II.5.9. Matching procedure for the effective potential with larger blocks $L = 8$ (full lines) and $L = 16$ (dotted). Details of the matching procedure are described in the caption of Figure II.5.8. The approach of the $\Delta\beta$-values obtained from this figure to the value predicted by perturbation theory $\Delta\beta_{per} \approx 0.12$ indicates that the renormalization group flow in the investigated β-region approaches a renormalized trajectory after three to four $L = 2$ block spin transformations.

Chapter III

Monte Carlo Investigation of Gaussian Block Spin Transformations Study of Locality Properties of Effective Hamiltonians for the Critical 2-Dimensional Ising Model

For effective Hamiltonians defined by a Gaussian block spin transformation it is easy to derive a Taylor expansion in the block spin fields ϕ. This is true for any type of fundamental variables which might be real variables (e.g. φ^4 theory) or obey certain constraints (Ising spins, O(N) spins or gauge variables). After a single renormalization group transformation the block spin variables are continuous and real. Thus in principle the Taylor expansion can be set up about an arbitrary reference field $\bar{\phi}$. The Taylor coefficients are truncated correlation functions in an auxiliary statistical mechanical system with fixed block spins $\bar{\phi}$. Since the width of the Gaussian factor is finite the block averages of the fundamental spins can fluctuate around the prescribed values of the block spins. Truncated correlations of these fluctuations determine the Taylor coefficients of the effective Hamiltonian.

The Taylor expansion about $\phi = \bar{\phi}$ is local if truncated correlations of block averages in the auxiliary system with background field $\bar{\phi}$ are of short range (exponential decay with range $\approx$ 1 block lattice constant). One cannot expect that $\mathcal{H}_{\text{eff}}(\phi)$ has good locality properties for all background fields $\bar{\phi}$. In analytical renormalization group studies this problem is known as the large field problem. The method described in this chapter allows a careful study of this problem also for strongly coupled models which are not yet accessible by analytical methods.

In Section III.1. Gaussian block spin transformations are defined. Taylor expansions of the effective Hamiltonian are derived with Taylor coefficients that can be computed by Monte Carlo simulations with fixed block spins. The large field problem is discussed.

Compared to simulations with strictly fixed block spins a Monte Carlo investigation of Gaussian block spin transformations is easier to do. Since the block averages can fluctuate, an algorithm can be used which updates single spin variables. The conditional probability distribution of a single spin is determined by the fundamental Hamiltonian and an additional quadratic interaction (due to the Gaussian factor) which couples the spin under consideration to the actual block average. In Section III.2. a heat bath algorithm for the Ising model is described.

I performed concrete Monte Carlo simulations for the 2-dimensional Ising model at the critical point. For block size $L = 2^n$, $n \leq 4$ and for three different values of the κ-parameter which determines the width of the Gaussian factor correlation functions of the block averages were measured for several constant background fields $\bar{\phi}$.

In Section III.3.A. results for the effective potential are presented. In Section III.3.B. we discuss Monte Carlo results for quadratic Taylor coefficients of the effective Hamiltonian. It turns out that Taylor expansions for the effective Hamiltonian of the 2-dimensional critical Ising model have bad locality properties if the expansion is about a reference field close to $\bar{\phi} = 0$.

This chapter is organized as follows:

III.1. Gaussian Block Spin Transformations, Taylor Expansions for the Effective Hamiltonian and the Large Field Problem

Linear Gaussian block spin transformations for lattice field theories are defined. A Taylor expansion for the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ in terms of the block spin fields is derived. The effective Hamiltonian can be expanded about arbitrary block spin configurations $\bar{\phi}$. The large field problem is discussed.

Let

$$Z = \int \prod_{x \in \Lambda} d\varphi(x)\, e^{-\mathcal{H}(\varphi)} \tag{1-1}$$

be the partition fuction of a statistical mechanical system with (dimensionless) random variables (spins) on a cubic d-dimensional lattice with lattice spacing 1. The $\varphi(x)$ can be e.g. real numbers, N-vectors, Ising or O(N) spins. $d\varphi$ is the Lebesgue measure on R^N for real random variables, the invariant sum over Z_2 for Ising variables or the uniform measure on S^{N-1} for O(N) spins. Let $\mathcal{H}(\varphi)$ be an arbitrary Hamiltonian.

A linear Gaussian block spin transformation onto a block lattice Λ' with lattice spacing L is defined by the effective Boltzmannian

$$e^{-\mathcal{H}_{\text{eff}}(\phi)} = \mathcal{N}_\kappa^{-1} \int \mathcal{D}\varphi\, e^{-\mathcal{H}(\varphi)} \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa |\phi(x) - b \sum_{z \in x} \varphi(z)|^2} \equiv \mathcal{Z}(\phi) \tag{1-2}$$

The normalization constant $\mathcal{N}_\kappa$ is chosen such that integration of the effective Boltzmannian over ϕ yields the original partition function (see Appendix B.1.):

$$Z = \int \prod_{x \in \Lambda'} d\phi(x)\, e^{-\mathcal{H}_{\text{eff}}(\phi)} \tag{1-3}$$

$d\phi$ - independent on the type of the fundamental variables - is the Lebesgue measure on R^N. A Gaussian renormalization group transformation depends on a positive parameter κ which

determines the width of the Gaussian factor. The parameter b defines normalization and wave function renormalization of the block spin fields. (In the neighbourhood of a renormalization group fixed point $b = L^{-\frac{1}{2}(d+2-\eta)}$, cf. Chapter I.)

κ and b cannot be chosen in an arbitrary way. If these parameters have been chosen for a block spin transformation with scale factor L then the κ- and b-values for arbitrary L are determined. This follows from the requirement that the composition of two successive block spin transformations with scale factors L_1 and L_2 should be exactly equivalent to a single transformation with a scale factor $L_1 \cdot L_2$. The composition rules for Gaussian block spin transformations are discussed in detail in Appendix B.1.

κ should not be chosen too small. Analytical studies [17] suggest that one should choose $\kappa \geq \pi^2$. This ensures that the fluctuation propagator Γ which mediates interactions in the auxiliary system with partition function $\mathcal{Z}(\phi)$ decays fast enough. Γ decays exponentially for all $\kappa > 0$, but for $\kappa \geq \pi^2$ the range of the fluctuation propagator is smaller than a block lattice spacing.

A problem associated with Gaussian block spin transformations is the wave function renormalization. Close to a renormalization group fixed point the parameter b is determined by the anomalous dimension η which in general is unknown. If there is no fixed point as for example in the 2-dimensional $O(N \geq 3)$ model one will define the wave function renormalization by a suitable renormalization condition for the effective potential or the kinetic term. In the case of the δ block spin (cf. Chapters II and IV) it is not necessary to know the wave function renormalization, because it is allowed to rescale the block spins afterwards and by this implement suitably chosen renormalization conditions. However, for Gaussian block spin transformations rescaling of the block spins is equivalent to a (block size dependent) change in the parameter κ which destroys the consistency of the renormalization group flow. As long as the effects of this can be expected to be small[1], the problem should be manageable. In any case a precise determination of the wave function renormalization will be more difficult as for the δ block spin. However, if the main interest is in locality properties of the effective Hamiltonian this is a problem of inferior importance. The concrete Monte Carlo simulations for this chapter were performed for the 2-dimensional Ising model. For this model η is exactly known.

A further difficulty which might hamper renormalization group studies with Gaussian block spins have their origin in *redundant operators* [4] which might show up for finite κ. Redundant operators have no influence on the physics of the model. In the field theoretic language they are operators whose expectation values vanish as a consequence of the field equations. The eigenvalues of redundant operators might be changed if the block spin definition is changed (e.g. by variation of κ), and if one is unfortunate one ore more of the redundant operators might become relevant.[2] If this happens the Hamiltonians $\mathcal{H}_{\text{eff}}^{(i)}$ will not converge to a fixed point $\mathcal{H}_{\text{eff}}^{*}$. Even if all redundant operators are irrelevant they might mask the irrelevant operator which dominates the leading corrections to scaling. We will not get into details here. Redundant operators are thoroughly discussed in [5] and in [6].

[1] This can be expected especially in more than two dimensions since there the anomalous dimension η usually is very small. Example: 3-dimensional Ising model, $\eta \approx 0.056$ [2].

[2] A *relevant* operator is an eigenoperator of the linearized renormalization group transformation with eigenvalue > 1. *Irrelevant* operators have eigenvalue < 1, the eigenvalue of a *marginal* operator exactly equals 1. See also Appendix C.2.

Gaussian block spin transformation also have merits. It will now be shown that they allow to easily derive Taylor expansions of $\mathcal{H}_{\text{eff}}(\phi)$ in the block spin fields.

For the following let us assume that φ is an N-vector field with components φ_α, $\alpha = 1...N$. Let $\bar{\phi}$ be an arbitrary reference configuration on the block lattice Λ'. For brevity we define

$$\psi(x) \equiv \phi(x) - \bar{\phi}(x), \quad \bar{\varphi}(x) \equiv b \sum_{z \in x} \varphi(z) \tag{1-4}$$

ψ parametrizes the deviation from the reference field $\bar{\phi}$, and $\bar{\varphi}$ is the rescaled block average. It is easy to see that

$$e^{-\mathcal{H}_{\text{eff}}(\phi)} = e^{-\frac{1}{2}\kappa \sum_x \psi(x)^2} \int \mathcal{D}\varphi \, e^{-\mathcal{H}(\varphi)} e^{-\frac{1}{2}\kappa \sum_x [\bar{\phi}(x) - \bar{\varphi}(x)]^2} e^{\kappa \sum_x \psi(x)[\bar{\varphi}(x) - \bar{\phi}(x)]} \tag{1-5}$$

and

$$e^{-[\mathcal{H}_{\text{eff}}(\phi) - \mathcal{H}_{\text{eff}}(\bar{\phi})]} = e^{-\frac{1}{2}\kappa \sum_x \psi(x)^2} \langle e^{\kappa \sum_x \psi(x)[\bar{\varphi}(x) - \bar{\phi}(x)]} \rangle_{\bar{\phi}} \tag{1-6}$$

with the $\bar{\phi}$-parametric expectation $\langle (\cdot) \rangle_{\bar{\phi}}$ defined by

$$\langle \mathcal{O}(\varphi) \rangle_{\bar{\phi}} \equiv \mathcal{Z}(\bar{\phi})^{-1} \int \mathcal{D}\varphi \, e^{-\mathcal{H}(\varphi)} e^{-\frac{1}{2}\kappa \sum_x [\bar{\phi}(x) - \bar{\varphi}(x)]^2} \mathcal{O}(\varphi) \tag{1-7}$$

This measure differs from the original measure by a quadratic term depending on the background field $\bar{\phi}$. Starting point for a Taylor expansion for $\mathcal{H}_{\text{eff}}(\phi)$ about $\phi = \bar{\phi}$ is the following equation:

$$\mathcal{H}_{\text{eff}}(\phi) = \mathcal{H}_{\text{eff}}(\bar{\phi}) + \frac{\kappa}{2} \sum_x \psi(x)^2 - \ln \langle e^{\kappa \sum_x \psi(x)[\bar{\varphi}(x) - \bar{\phi}(x)]} \rangle_{\bar{\phi}} \tag{1-8}$$

The (formal) expansion of the logarithm leads to a sum over truncated correlation functions:

$$\begin{aligned} &\ln \langle e^{\kappa \sum_x \psi(x)[\bar{\varphi}(x) - \bar{\phi}(x)]} \rangle_{\bar{\phi}} \\ &= \sum_{n \geq 1} \frac{1}{n!} \langle \left(\kappa \sum_x \psi(x)[\bar{\phi}(x) - \bar{\varphi}(x)] \right)^n \rangle_{\bar{\phi}}^T \\ &= \sum_{n \geq 1} \frac{\kappa^n}{n!} \sum_{x_1} \cdots \sum_{x_n} \langle \prod_{i=1}^{n} [\bar{\varphi}_{\alpha_i}(x_i) - \bar{\phi}_{\alpha_i}(x_i)] \rangle_{\bar{\phi}}^T \cdot \prod_{j=1}^{n} \psi_{\alpha_j}(x_j) \end{aligned} \tag{1-9}$$

Summation over repeated vector indices is understood. If we define

$$\mathcal{H}_{\text{eff}}(\phi) = \mathcal{H}_{\text{eff}}(\bar{\phi}) + \sum_{n \geq 1} \frac{1}{n!} \sum_{x_1} \cdots \sum_{x_n} h_{\alpha_1 \ldots \alpha_n}(x_1, \ldots, x_n | \bar{\phi}) \cdot \psi_{\alpha_1}(x_1) \ldots \psi_{\alpha_n}(x_n) \tag{1-10}$$

we find the following formula for the h-kernels:

$$h_{\alpha_1 \ldots \alpha_n}(x_1, \ldots, x_n | \bar{\phi}) = \kappa \cdot \delta_{n,2}\, \delta_{\alpha\beta}(x_1, x_2) - \kappa^n \langle \prod_{i=1}^{n} [\bar{\varphi}_{\alpha_i}(x_i) - \bar{\phi}_{\alpha_i}(x_i)] \rangle_{\bar{\phi}}^T \tag{1-11}$$

For $n = 1$:

$$h_\alpha(x|\bar{\phi}) = \kappa [\bar{\phi}_\alpha(x) - \langle \bar{\varphi}_\alpha(x) \rangle_{\bar{\phi}}] \tag{1-12}$$

For $n \geq 2$ the truncated correlation functions remain unchanged if the $\bar{\phi}(x)$ are not subtracted. Thus

$$h_{\alpha_1 \ldots \alpha_n}(x_1, \ldots, x_n | \bar{\phi}) = \kappa \cdot \delta_{n,2}\, \delta_{\alpha\beta}(x_1, x_2) - \kappa^n \langle \bar{\varphi}_{\alpha_1}(x_1) \ldots \bar{\varphi}_{\alpha_n}(x_n) \rangle_{\bar{\phi}}^T \tag{1-13}$$

The following considerations shall give a rough picture of what is known about analyticity properties of effective Hamiltonians from rigorous renormalization group studies of weakly coupled theories [18]. $\mathcal{H}_{\text{eff}}(\phi)$ has good locality properties to each order of perturbation theory. This is due to the fact that the fluctuation propagator which mediates perturbative excitations of the auxiliary system decays rapidly with distance. However, beyond perturbation theory there is a large field problem. For a given block spin configuration regions of the lattice can exist where the effective Hamiltonian becomes very large (locally). In order to understand the origin of this problem we first consider the effective Boltzmannian

$$e^{-\mathcal{H}_{\text{eff}}(\phi)} = \int \mathcal{D}\varphi\, e^{-\mathcal{H}(\varphi)} \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa |\phi(x) - b \sum_{z \in x} \varphi(z)|^2} \equiv \mathcal{Z}(\phi) \tag{1-14}$$

It is useful to consider $\mathcal{Z}(\phi)$ as a function of *complex* variables $\phi(x)$, $x \in \Lambda'$. For the following let us assume that the fundamental random variables φ take values on a compact space (examples: O(N) model, pure gauge theory). Then $\mathcal{Z}(\phi)$ is an *entire* function[1] of the complex variables $\phi(x)$. This is a consequence of the the following facts:

1. The integrand depends on ϕ only through the Gaussian factors. These factors are entire functions of $\phi(x)$.
2. The φ-variables are integrated over a compact space. By this no singularities can be generated.
3. "Reasonable" Hamiltonians $\mathcal{H}(\varphi)$ have a lower bound on the domain of φ. Therefore the fundamental Boltzmannian $e^{-\mathcal{H}(\varphi)}$ has an upper bound and cannot generate singularities.

[1] A function $f : \mathcal{C}^N \to \mathcal{C}$ is called *holomorphic* in an open subset $U \subseteq \mathcal{C}^N$ if each point $z_0 \in U$ has an open neighbourhood in which f can be represented by a convergent power series. For *entire*-functions $U = \mathcal{C}^N$. A theorem of the theory of several complex variables says that holomorphy of f in each single variable implies holomorphy of f in a corresponding open subset of $\mathcal{C}^N$ [19].

However, $\mathcal{H}_{\text{eff}}(\phi) = -\ln \mathcal{Z}(\phi)$ is not necessarily an entire function. $\mathcal{Z}(\phi)$ might have zeros for complex ϕ. (For real ϕ strictly $\mathcal{Z}(\phi) > 0$.) At these zeros the effective Hamiltonian diverges. Of course, one cannot expect the existence of local Taylor expansions in the neighbourhood of poles. If the zeros of the effective Boltzmannian are close to the real axis they will badly affect the locality properties of $\mathcal{H}_{\text{eff}}(\phi)$.

In analytical renormalization group studies for a given (real) block spin configuration ϕ the block lattice is divided into small field region and large field region [18]. The small field region is defined as the set of all sites $x \in \Lambda'$ in whose neighbourhood the energy density associated with $\mathcal{H}_{\text{eff}}(\phi)$ is small. The large field region consists of all sites x which do not belong to the small field region. A more precise precise meaning shall be given to this in the following. Consider a representation of $\mathcal{H}_{\text{eff}}(\phi)$ as a sum over contributions which are associated with subsets $X \subseteq \Lambda'$:

$$\mathcal{H}_{\text{eff}}(\phi) \equiv \sum_{\emptyset \neq X \subseteq \Lambda'} \mathcal{H}'(X|\phi) \tag{1-15}$$

$\mathcal{H}'(X|\phi)$ is a contribution to $\mathcal{H}_{\text{eff}}(\phi)$ which has support on X, i.e. depends on ϕ only through $\phi(x)$ with $x \in X$. The $\mathcal{H}'(X|\phi)$ are uniquely determined if effective Hamiltonians $\mathcal{H}_{\text{eff}}(Y|\phi)$ are defined for lattices Y of arbitrary shape and size. One requires that $\mathcal{H}_{\text{eff}}(Y|\phi)$ depends on ϕ only through $\phi(y)$ with $y \in Y$. A further condition is that $\mathcal{H}_{\text{eff}}(\Lambda'|\phi) = \mathcal{H}_{\text{eff}}(\phi)$. By the help of the Möbius inversion formula (see for example [15]) one can express the $\mathcal{H}'(X|\phi)$ in terms of the $\mathcal{H}_{\text{eff}}(Y|\phi)$ with $Y \subseteq X$. It turns out that[1]

$$\mathcal{H}'(X|\phi) = \sum_{\emptyset \neq Y \subseteq X} (-1)^{|X| - |Y|}\, \mathcal{H}_{\text{eff}}(Y|\phi) \tag{1-16}$$

A possibility to define the $\mathcal{H}_{\text{eff}}(Y|\phi)$ in the case of a Gaussian renormalization group transformation is the following: Let $\bar{\phi}$ be a block spin configuration such that $\mathcal{H}_{\text{eff}}(\phi)$ is minimal for $\phi = \bar{\phi}$. For a ferromagnetic system the minimum of $\mathcal{H}_{\text{eff}}(\phi)$ coincides with the minimum of the effective potential $\mathcal{V}_{\text{eff}}(\phi)$ since any "gradient" pressed into the constant $\bar{\phi}$-configuration will cost energy. $\bar{\phi}$ is not necessarily uniquely determined. E.g., a minimum of the effective potential at $\bar{\phi} \neq 0$ is degenerate with respect to the symmetry of the model (reflections for the Ising model, rotations for the O(N) model). For weakly coupled models without spontaneously broken symmetry one will choose $\bar{\phi} = 0$.

By adding a suitably chosen constant the effective Hamiltonian can be normalized such that $\mathcal{H}_{\text{eff}}(\bar{\phi}) = 0$.[2] This is equivalent to a redefinition of the effective Boltzmannian

$$\begin{aligned} e^{-\mathcal{H}_{\text{eff}}(\phi)} &= \frac{\int \mathcal{D}\varphi\, e^{-\mathcal{H}(\varphi)} \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa |\phi(x) - \bar{\varphi}(x)|^2}}{\int \mathcal{D}\varphi\, e^{-\mathcal{H}(\varphi)} \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa |\bar{\phi}(x) - \bar{\varphi}(x)|^2}} \\ &= \langle \prod_{x \in \Lambda'} e^{-\frac{1}{2}\kappa [(\phi(x) - \bar{\varphi}(x))^2 - (\bar{\phi}(x) - \bar{\varphi}(x))^2]} \rangle_{\bar{\phi}} \end{aligned} \tag{1-17}$$

[1] $|X|$ denotes the number of points in X.

[2] Sites x with $\phi(x)$ close to $\bar{\phi}$ therefore *per definitionem* are in the small field region.

One now defines

$$e^{-\mathcal{H}_{\rm eff}(Y|\phi)} = \langle \prod_{x\in Y} e^{-\frac{1}{2}\kappa[(\phi(x)-\varphi(x))^2-(\bar\phi(x)-\varphi(x))^2]} \rangle_{\bar\phi} \tag{1-18}$$

Obviously $\mathcal{H}_{\rm eff}(Y|\bar\phi) = 0$ for all $Y \subseteq \Lambda'$. We now define an "energy density" $\bar{\mathcal{H}}(x|\phi)$ such that

$$\mathcal{H}_{\rm eff}(\varphi) = \sum_{x\in\Lambda'} \bar{\mathcal{H}}(x|\phi) \tag{1-19}$$

The relation with $\mathcal{H}'(X|\phi)$ is given by

$$\bar{\mathcal{H}}(x|\phi) = \sum_{X: x\in X} |X|^{-1}\, \mathcal{H}'(X|\phi) \tag{1-20}$$

Small field region and large field region can now be defined more precisely:

$$\begin{aligned} &\textit{small field region} \equiv \{x\in\Lambda' \,:\, \bar{\mathcal{H}}(x|\phi) < \gamma, \quad \gamma \gg 1\} \\ &\textit{large field region} \equiv \Lambda' - \textit{small field region} \end{aligned} \tag{1-21}$$

On the basis of rigorous studies for weakly coupled models [*18*] one expects the following picture for a "generic" block spin configuration ϕ: Nearly all sites $x \in \Lambda'$ will belong to the small field region. The complement (the large field region) can be decomposed into connected parts which are called large field islands. These islands are typically small (typical size at most a few block lattice constants). Big large field islands are rare.

In the small field regions the contributions to $\mathcal{H}'(X|\phi)$ are small if either the number of points in X is large or if X contains widely separated points.[1] This is the precise formulation of the statement that the effective Hamiltonian has good locality properties in the small field region.

We now proceed to the discussion of analyticity properties of $\mathcal{H}_{\rm eff}(\phi)$ in the small field region. The essential point will be that in the small field region the contributions $\mathcal{H}'(X|\phi)$ will become very small if X has a large "tree length". It follows that the sum for the effective Hamiltonian in Eq. (1-15) can be truncated. Thus (up to translations) one needs to consider only a finite number of sets X. The analyticity of the truncated effective Hamiltonian follows from the analyticity of the finite number of contributions $\mathcal{H}'(X|\phi)$: The quantity $\mathcal{H}'(X|\phi)$ is again composed from a finite number of contributions $\mathcal{H}_{\rm eff}(Y|\phi)$, $Y \subseteq X$ (see equation (1-16)). We now consider the partition functions $\mathcal{Z}(Y|\phi) \equiv e^{-\mathcal{H}_{\rm eff}(Y|\phi)}$. These are entire functions of the variables $\phi(y)$, $y \in Y$, and strictly positive for real ϕ. The number and position of the zeros of $\mathcal{Z}(Y|\phi)$ will depend on Y. Since for given X we have to consider only a finite number of subsets Y a common complex neighbourhood $\mathcal{O}$ of $\phi = \bar\phi$ will exist such that $\mathcal{Z}(Y|\phi)$ is free of zeros for all $Y \subseteq X$ and $\phi \in \mathcal{O}$. As a consequence $\mathcal{H}_{\rm eff}(Y|\phi) = -\ln \mathcal{Z}(Y|\phi)$ will

[1] The relevant quantity which determines the decay is the length of the shortest tree which connects all sites in X.

be holomorphic on $\mathcal{O}$. The same will be true for $\mathcal{H}'(X|\phi) = \sum_{Y\subseteq X}(-1)^{|X|-|Y|}\mathcal{H}_{\rm eff}(Y|\phi)$. This implies analyticity of the truncated sum of contributions $\bar{\mathcal{H}}'(X|\phi)$ which defines an (approximate) effective Hamiltonian, for $\phi \in \mathcal{O}$ and for lattices Λ' of arbitrary size.

III.2. Monte Carlo Simulations with Fixed Gaussian Block Spins

Monte Carlo simulations with fixed Gaussian block spins allow a "single spin updating". A heat bath algorithm for the Ising model is described in some detail.

For a given block spin field ϕ we want to generate a sequence of Ising configurations s which are distributed according to

$$\text{prob}(s) \propto e^{\beta\sum_{<v,w>} s(v)s(w)} \prod_{x\in\Lambda'} e^{-\frac{1}{2}\kappa[\phi(x)-b\sum_{z\in x} s(z)]^2} \tag{2-1}$$

prob(s) defines a conditional probability distribution for a single spin $\sigma \equiv s(v)$. Let v be a site in block x and $\phi(x) \equiv \chi$. Then

$$\text{prob}(\sigma) \propto e^{\beta t\sigma}\cdot e^{-\frac{1}{2}\kappa[\hat\chi - b\sigma]^2} \tag{2-2}$$

Let us define

$$t \equiv \sum_{<v,w>} s(w), \quad \hat\chi \equiv \chi - b\sum_{x\ni z\neq v} s(z) \tag{2-3}$$

Removing factors independent on σ one finds

$$\text{prob}(\sigma) \propto e^{[\beta t + \kappa b\hat\chi]\,\sigma} \tag{2-4}$$

In addition to the magnetic field βt generated by the 2d nearest neighbours σ will be affected by a magnetic field $\kappa b\hat\chi$ which is determined by the block spin ϕ and the average of the other spins in the block.[1]

The computation of $\hat\chi$ requires little effort if the block sums

$$F(x) \equiv \sum_{z\in x} s(z) \tag{2-5}$$

are stored and actualized after each update. Since we want to measure block averages it is advantageous if one needs not to recompute the block sums after each sweep. For the Ising model it is suggestive to use a heat bath algorithm. We define an effective magnetic field

[1] A vectorization of the algorithm is hampered by the nonlocal interaction of the spins. On the basis of a "checkerboard" on the block lattice to remove any kind of dependencies one obtains a maximal vector length of $|\Lambda'|/2$.

$$h_{\text{eff}} \equiv \beta t + \kappa b\tilde{\chi} \tag{2-6}$$

The probability distribution for σ is easily normalized:

$$\text{prob}(\sigma = +1) = [1 + e^{-2h_{\text{eff}}}]^{-1} \tag{2-7}$$

The possible values of prob($\sigma = +1$) can be stored in the computer before the Monte Carlo simulation. A heat bath updating for a spin variable σ consists of the following steps:

(1) Determine the sum of nearest neighbours t and $\tilde{F}(x) \equiv F(x) - \sigma$.

(2) Read prob($\sigma = +1$) from a table stored in the computer.

(3) Generate a random number $0 < rnd < 1$. If $rnd <$ prob($\sigma = +1$) let $\sigma = +1$. Else let $\sigma = -1$.

(4) If σ was changed update the block sum $F(x)$ accordingly.

III.3. Monte Carlo Results for the 2-Dimensional Ising Model at the Critical Point

Results of Monte Carlo simulations of the critical Ising model in two dimensions with fixed Gaussian block spins are presented. Results for the effective potential (Section A) and for quadratic Taylor coefficients (Section B) are discussed.

Parameters of the Monte Carlo experiment:
For block size $L = 2^n$, $n = 1, 2, 3, 4$ and for three values of κ (see below) always 15 Monte Carlo runs were performed: For each value of the constant background field $\phi = \{0.0, 0.1, ..., 1.4\}$ 250×100 heat bath updating sweeps with $\beta_c = 0.440687$ (as described in Section III.2.) were done. After each sweep several correlation functions of the block averages were measured. Averaging over 100 succesive sweeps was done during the Monte Carlo run. So for any configuration of the parameters (L, ϕ, κ) and for each observable we have 250 data points.

blocks	block lattice
2×2	25×25
4×4	15×15
8×8	10×10
16×16	10×10

The total CPU for this study was about 100 hours on the scalar computer [49]. The mean CPU needed for a single heat bath update was approximately 10 μsec.

b-parameter: The b-parameter appearing in the Gaussian block spin definition was chosen according to the formula $b = L^{-\frac{1}{2}(4-\eta)}$ with $\eta = 0.25$. The following table shows the coefficients b_n for block size $L = 2^n$. For a comparison the corresponding b-values for $\eta = 0$ are also displayed.

	$b_1 \equiv b$	b_2	b_3	b_4
$\eta = 0.25$	0.2726	$7.4325 \cdot 10^{-2}$	$2.0263 \cdot 10^{-2}$	$5.5243 \cdot 10^{-3}$
$\eta = 0.00$	0.2500	$6.2500 \cdot 10^{-2}$	$1.5625 \cdot 10^{-2}$	$3.9063 \cdot 10^{-3}$

κ-parameter: It is shown in Appendix B.1. that for a consistent renormalization group flow it is necessary that κ depends on L. It turns out that for block size $L = 2^n$ in two dimensions

$$\frac{\kappa_n}{\kappa} = \frac{1 - (4b^2)}{1 - (4b^2)^n} \tag{3-1}$$

$\kappa \equiv \kappa_1$ is the parameter for a $L = 2$ block spin transformation. The following table displays the κ_n used in this Monte Carlo study.

$\kappa_1 \equiv \kappa$	κ_2	κ_3	κ_4	κ_∞	π^2
6.0000	4.6250	4.3300	4.2494	4.2162	9.8696
12.0000	9.2500	8.6599	8.4988	8.4324	9.8696
18.0000	13.8750	12.9900	12.7482	12.6486	9.8696

After each sweep the values of eight observables were measured: $\bar{s}(x)$, $\bar{s}(x)^2$ and $\bar{s}(x)\bar{s}(y)$ with $|x - y| \leq 3$. Because of the constant background fields $\bar{\phi}$ the expectation values of these quantities are invariant under translations in the block lattice.

name	observable	$\|x - y\|$	contributions/volume
c_0	$\bar{s}(x)$	0	1
c_{00}	$\bar{s}(x)^2$	0	1
c_{01}	$\bar{s}(x)\bar{s}(y)$	1	2
c_{02}	$\bar{s}(x)\bar{s}(y)$	$\sqrt{2}$	2
c_{03}	$\bar{s}(x)\bar{s}(y)$	2	2
c_{04}	$\bar{s}(x)\bar{s}(y)$	$\sqrt{5}$	4
c_{05}	$\bar{s}(x)\bar{s}(y)$	$\sqrt{8}$	2
c_{06}	$\bar{s}(x)\bar{s}(y)$	3	2

The name c_{0n} means that y is an n-th neighbour of x.

The following little table shows the positions of the n-th neighbours of the origin for $n \leq 6$.

6			
3	4	5	
1	2	4	
0	1	3	6

From the averages of the quantities c one can obtain Monte Carlo estimates for the Taylor coefficients

$$h(x|\phi) = \kappa[\phi - \langle \bar{s}(x) \rangle_\phi] \tag{3-2}$$

and

$$h(0,x|\phi) = \kappa\,\delta(0,x) - \kappa^2 \langle \bar{s}(0)\bar{s}(x) \rangle_\phi^T \tag{3-3}$$

In order to determine statistical errors the data sample was divided in 10 groups. The errors were then obtained from the standard deviation over the 10 subsamples. The connected parts of the 2-point functions were determined separateley within each subsample.

Part of the numerical results for the h-kernels is listed in Appendix B.3.

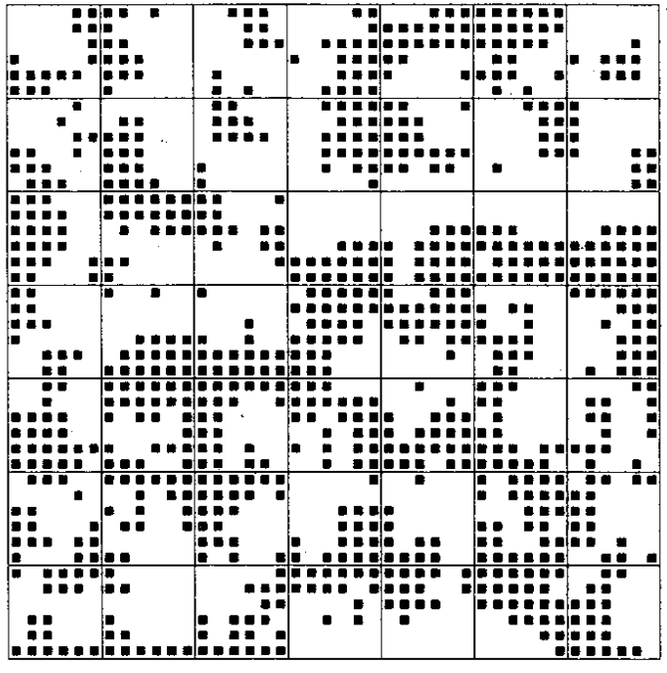

Figure III.3.1. A section of a typical Ising lattice with background field $\bar{\phi} = 0$. The block size is $L = 6$, the Gaussian parameter is $\kappa = 12$ and $\beta = \beta_c$. The black squares represent spins $s = +1$, the corresponding white sites are occupied by spins with $s = -1$. The figure shows that for $\kappa = 12$ the block averages considerably fluctuate away from zero. This is less surprising if one recognizes that $\bar{\phi} = 0$ is not a generic background field. The effective potential (see Figures III.3.4. ff.) prefers block averages $\neq 0$. The truncated correlations of the fluctuations determine the Taylor coefficients of the effective Hamiltonian. For $\bar{\phi} = 0$ these correlations decay only slowly with distance. A Taylor expansion of $\mathcal{H}_{eff}(\phi)$ about $\phi = 0$ therefore does not have good locality properties (see Section III.3.B.).

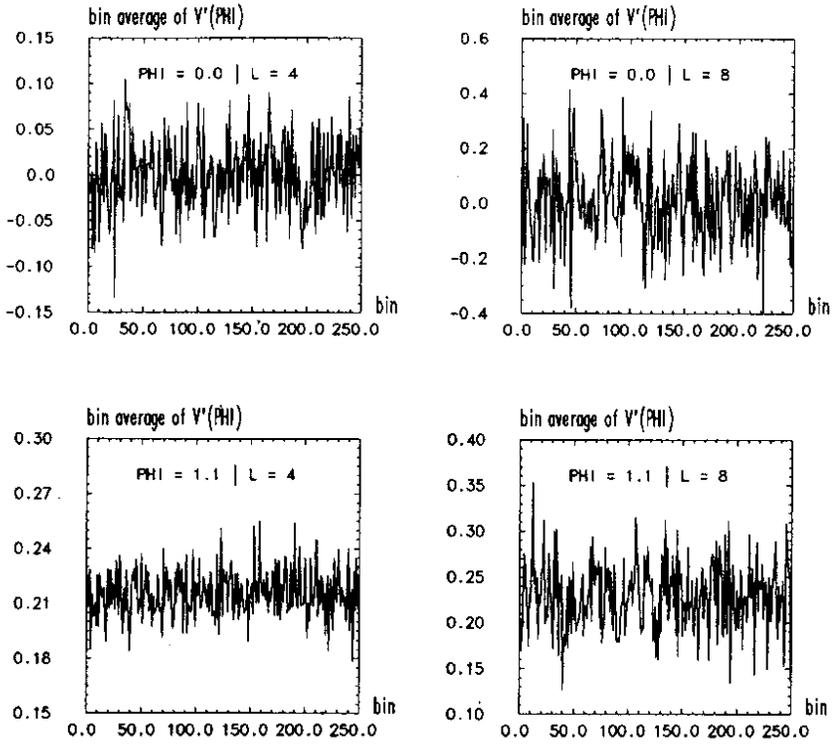

Figure III.3.2. Scatterplot for the bin averages $\kappa[\phi(x) - \langle\bar{s}(x)\rangle_\phi]$. The parameter of the Gaussian is $\kappa = 12$. For constant block spin ϕ this quantity is the derivative of the effective potential with respect to ϕ. A single dot in the figur represents the average over 100 successive sweeps. The figur shows bin averages for two special situations. $\phi = 0$ is a very unlikely configuration (large field). Here one has to be aware of critical slowing down. In particular for large blocks ($L = 8$) strong correlations in the data are obvious. $\phi = 1.1$ is close to the minimum of the effective potential. Here one expects the best behaviour. Nevertheless, autocorrelations can be observed.

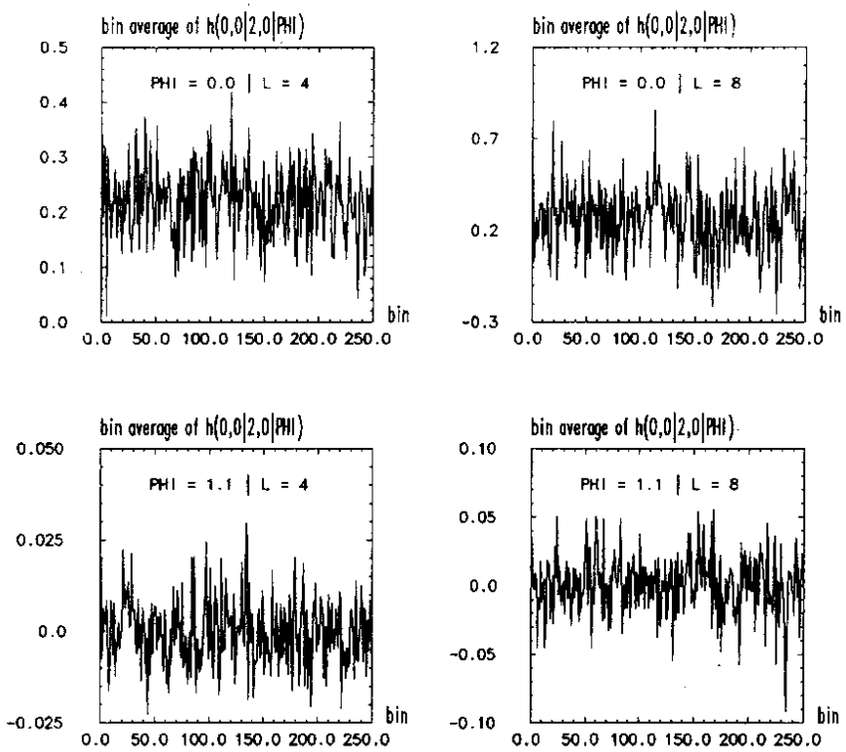

Figure III.3.3. Scatterplot for the bin averages $-\kappa^2\langle\bar{s}(x)\bar{s}(y)\rangle_\phi$ with $|x - y| = 2$. The Gaussian parameter is $\kappa = 12$. ϕ is a constant block spin background field. A single dot in the figure represents an average over 100 succesive sweeps. The performance is not obviously worse than for the local observable $\kappa[\phi - \langle\bar{s}(x)\rangle_\phi]$ (Figure III.3.2.).

For the computation of averages the data from the first 50 bins (= 5000 sweeps) were discarded. In order to determine statistical errors the 200 bins left were divided into 10 groups. The errors (= standard deviations of the mean values of the bin averages) are stable under increasing the bin size.

III.3.A. Effective Potential

For Gaussian block spin transformations the effective potential $\mathcal{V}_{\rm eff}(\phi)$ is easy to compute. $(\partial/\partial\phi)\mathcal{V}_{\rm eff}(\phi)$ can directly be determined by Monte Carlo simulations with constant blockspin ϕ. In contrast to the method proposed in Chapter II it is not necessary to perform simulations for a whole sequence of β-values. Results are presented for the renormalization group flow of the effective potential on the critical surface of the 2-dimensional Ising model.

Let

$$e^{-V_{\rm eff}(\phi)} \equiv e^{-\mathcal{H}_{\rm eff}(\phi)|_{\phi=\rm const}} = \sum_s e^{-\beta\mathcal{H}(s)} e^{-\frac{1}{2}\kappa\sum_x[\phi-\bar{s}(x)]^2} \tag{3-4}$$

Then

$$\frac{\partial}{\partial\phi}V_{\rm eff}(\phi) = \kappa\sum_x\langle\phi-\bar{s}(x)\rangle_{\phi=\rm const} \tag{3-5}$$

The expecation value $\langle(\cdot)\rangle_\phi$ is translationally invariant for constant block spin. Thus for $\mathcal{V}_{\rm eff}(\phi) \equiv V_{\rm eff}(\phi)/|\Lambda'|$

$$\frac{\partial}{\partial\phi}\mathcal{V}_{\rm eff}(\phi) = \kappa[\phi-\langle\bar{s}(x)\rangle_{\phi=\rm const}] \tag{3-6}$$

$\mathcal{V}_{\rm eff}(\phi)$ can be determined by integration over ϕ. We define the integration constant such that the effective potential is zero at its minimum.

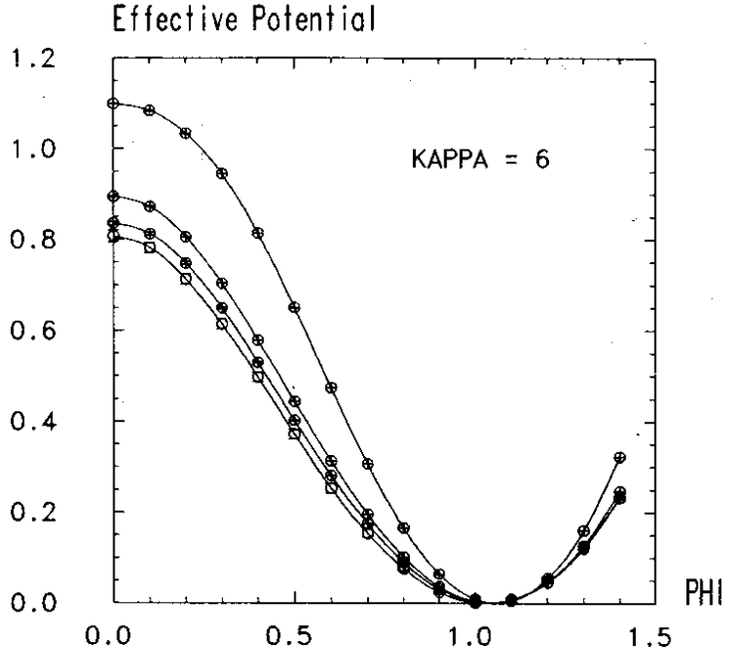

Figure III.3.4. The effective potential for $\kappa = 6$. The figure shows the flow of the potential with decreasing UV-cutoff. From top to bottom the curves belong to block size $L = 2, 4, 8, 16$. The results were obtained by integration of $(\partial/\partial\phi)\mathcal{V}_{\rm eff}(\phi) = \kappa[\phi - \langle\bar{s}(x)\rangle_\phi]$ over ϕ. The Monte Carlo data for the derivative of the potential for $\phi = 0.0/0.1/.../1.4$ were interpolated with splines and then integrated over ϕ. The integration constant was chosen such that the effective potential vanishes at its minimum. In order to determine statistical errors the data were divided into 10 groups. The potential was determined for each group separately. The error bars in the figure are given by the standard deviation of the average effective potential over the 10 groups.

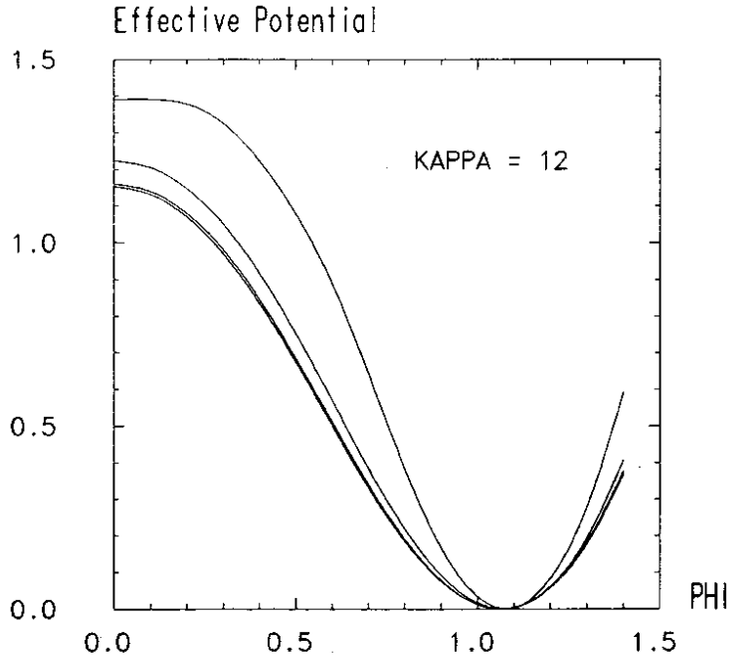

Figure III.3.5. The effective potential for $\kappa = 12$ and $L = 2, 4, 8, 16$ (top - bottom). Compared with $\kappa = 6$ the convergence to the fixed point is much better. The statistical errors are of the same order as for $\kappa = 6$. The potentials for $L = 8$ and $L = 16$ can hardly be separated within the statistical uncertainty.

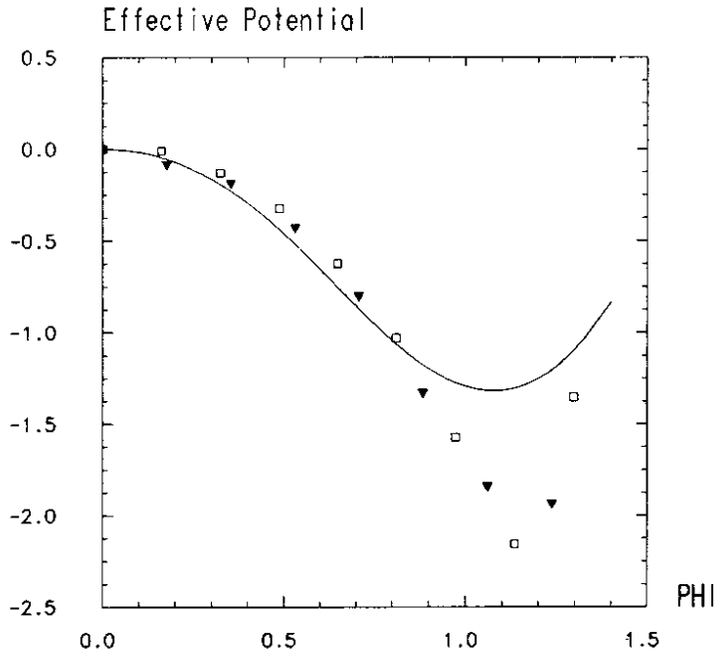

Figure III.3.6. The fixed point potential for $\kappa = 18$ compared with the fixed point potential for the δ block spin ($\kappa = \infty$). The full line shows the spline interpolation for the $L = 16$-potential with $\kappa = 18$. The dots represent the potential with Kronecker-δ block spin (see Chapter II, Figure II.4.5.). The sqares belong to $L = 8$, the triangles to $L = 16$.

This picture clearly shows that the renormalization group scenario strongly depends on the choice of the block spin. For the δ block spin the fixed point potential is nearly as twice as deep as for the Gaussian block spin with $\kappa = 18$.

III.3.B. 2-Point Taylor Kernels and Locality

Locality properties of quadratic Taylor kernels for the effective Hamiltonian of the critical 2-dimensional Ising model are investigated. A comparison of "truncated zero momentum sums" of 2-point kernels with the second derivative of the potential shows convergence problems of a Taylor expansion about $\bar{\phi} = 0$. It will be shown that an approximation for the effective Hamiltonian in the form $\mathcal{H}_{\text{eff}}(\phi) = \frac{\rho}{2}\sum_x \phi(x)[-\Delta\phi](x) + \sum_x \mathcal{V}_{\text{eff}}[\phi(x)]$ is not possible.

If constant fields $\bar{\phi}$ and ψ are inserted into the Taylor expansion

$$\mathcal{H}_{\text{eff}}(\phi) = \mathcal{H}_{\text{eff}}(\bar{\phi}) + \sum_{n\geq 1}\frac{1}{n!}\sum_{x_1}\cdots\sum_{x_n} h(x_1,\ldots,x_n|\bar{\phi})\cdot\psi(x_1)\ldots\psi(x_n) \tag{3-7}$$

one obtains an expansion for the effective potential in powers of $\psi = \phi - \bar{\phi}$:

$$\begin{aligned}\mathcal{V}_{\text{eff}}(\phi) &= \mathcal{V}_{\text{eff}}(\bar{\phi}) + |\Lambda'|^{-1}\sum_{n\geq 1}\frac{\psi^n}{n!}\sum_{x_1}\cdots\sum_{x_n} h(x_1,\ldots,x_n|\bar{\phi}) \\ &= \mathcal{V}_{\text{eff}}(\bar{\phi}) + \sum_{n\geq 1}\frac{\psi^n}{n!}\sum_{x_2}\cdots\sum_{x_n} h(0,x_2,\ldots,x_n|\bar{\phi})\end{aligned} \tag{3-8}$$

We have used the translational invariance of the h-kernels for constant background field $\bar{\phi}$. We find

$$\left(\frac{\partial}{\partial\bar{\phi}}\right)^n \mathcal{V}_{\text{eff}}(\phi) = \sum_{x_2}\cdots\sum_{x_n} h(0,x_2,\ldots,x_n|\phi) \tag{3-9}$$

If the derivates of $\mathcal{V}_{\text{eff}}(\phi)$ are already known (from independent calculations, see Section III.3.A.) these relations can be used to investigate the convergence of partial sums of the h-coefficients to the n-th derivative of $\mathcal{V}_{\text{eff}}(\phi)$. The figures on the two following pages show such an investigation for the 2-point kernels $h(0,x|\phi)$. The second derivative of $\mathcal{V}_{\text{eff}}(\phi)$ was obtained from the Monte Carlo results for $(\partial/\partial\phi)\mathcal{V}_{\text{eff}}(\phi)$ by differentiating the interpolation splines. On the other hand the partial sums $\sum_{|x|^2\leq d} h(0,x|\phi)$ with $d \leq 9$ can be determined from the Monte Carlo data for $h(0,x|\phi)$.

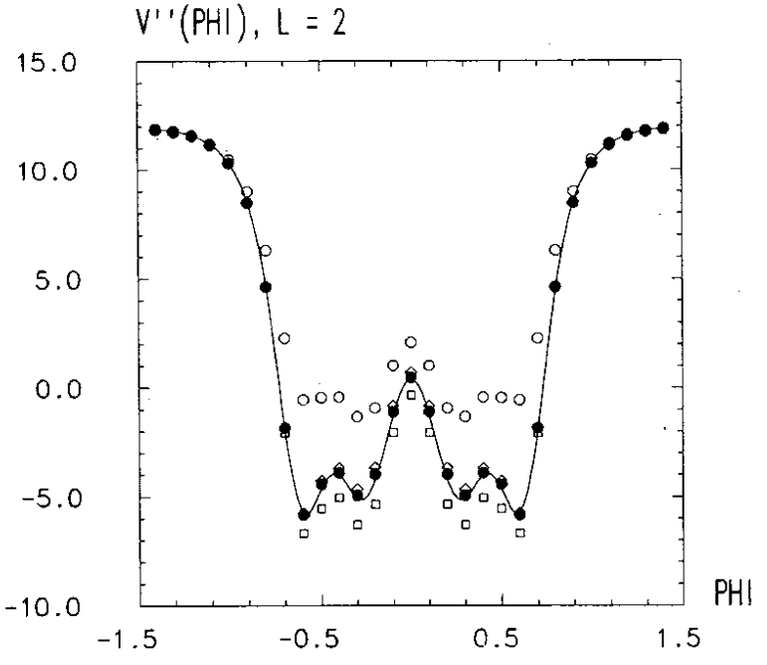

Figure III.3.7. Locality test for the quadratic Taylor kernels for constant background fields ϕ. The block size is $L = 2$, the Gaussian parameter $\kappa = 12$. The full line was obtained by differentiating the spline interpolation curve for the Monte Carlo data $\mathcal{V}'_{\text{eff}}(\phi) = \kappa[\phi - \langle\bar{s}(x)\rangle_\phi]$. The other symbols show partial sums $P_d(\phi) \equiv \sum_{|x|^2\leq d} h(0,x|\phi)$.

$P_0(\phi)$: circles

$P_2(\phi)$: squares

$P_5(\phi)$: diamonds

$P_9(\phi)$: dots

The partial sums converge alternatingly to $\mathcal{V}''_{\text{eff}}(\phi)$. The convergence is fast in a neighbourhood of $\phi = 1.0$ but rather slow for small ϕ. This phenomenon becomes more pronounced for larger blocks, cf. figures on the next page.

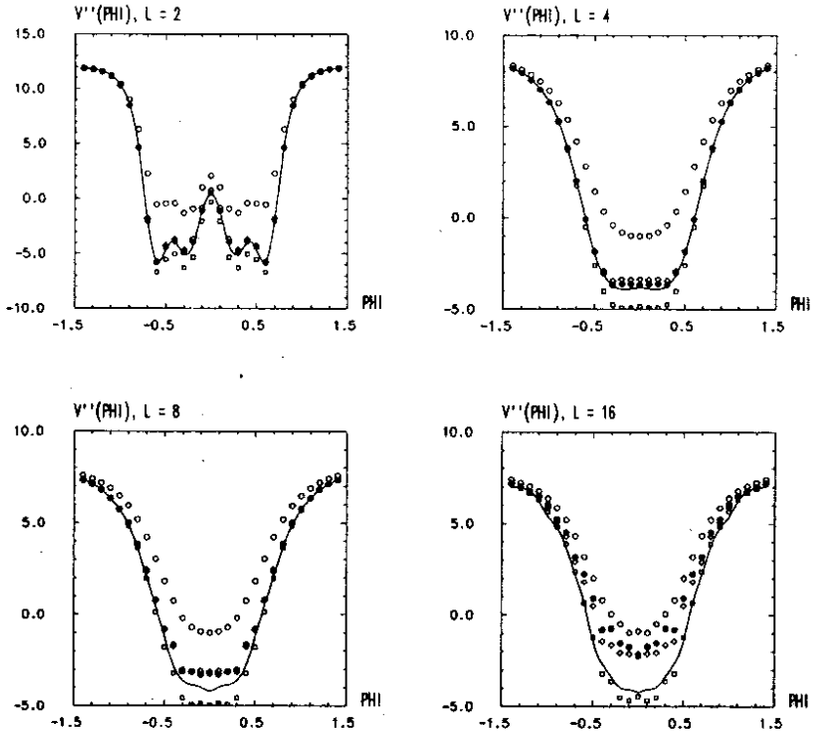

Figure III.3.8. Locality test for several block sizes. The Gaussian parameter is again $\kappa = 12$. As in Figure III.3.7. the full lines show derivatives of splines for the Monte Carlo observable $\mathcal{V}'_{\text{eff}}(\phi)$. The other symbols again show partial sums of $\sum_{x\in\Lambda'} h(0,x|\phi)$. The meaning of the symbols is the same as in Figure III.3.7.

With increasing block size an increasingly worse convergence of the partial sums for small ϕ can be observed. Here the effective Hamiltonian becomes very nonlocal. A truncation of the quadratic interaction such that all Taylor coefficients $h(x,y)$ with $|x-y| \geq 3$ are neglected is therefore not possible. It is important to recognize that this problem is not due to statistical errors. Its origin is not a too small κ. For $\kappa = 18$ the picture is essentially the same.

In the following we will study the effective Hamiltonian in the approximation

$$\mathcal{H}_{\text{eff}}(\phi) = \sum_x \mathcal{V}_{\text{eff}}[\phi(x)] + \frac{1}{2}\sum_x \sum_y T(x,y|\bar{\phi})\cdot\psi(x)\psi(y) + R(\psi) \tag{3-10}$$

We choose constant background fields $\bar{\phi}$. The remainder $R(\psi)$ is $O(\psi^3)$. All terms but the potential are required to vanish for constant ψ. Thus for the "kinetic operator" T

$$T(x,y|\bar{\phi}) = h(x,y|\bar{\phi}) - \{\sum_z h(0,z|\bar{\phi})\}\cdot\delta_{x,y} \tag{3-11}$$

It is easy to verify that $\sum_y T(x,y|\bar{\phi}) = 0$. The Fourier transform of T is given by

$$\begin{aligned}\hat{T}(p|\bar{\phi}) &= \sum_{x\in\Lambda'} e^{ipx}\, T(0,x|\bar{\phi}) \\ &= \sum_{x\in\Lambda'} \cos(px)\, T(0,x|\bar{\phi})\end{aligned} \tag{3-12}$$

For a block lattice Λ' with infinite extension p can vary continuously on $[0,2\pi)\times[0,2\pi)$. Only contributions $\propto \cos(px)$ appear because $T(0,x|\phi)$ is an even function of x.

$\hat{T}$ can be expressed in term of $\hat{h}$ as follows:

$$\hat{T}(p|\bar{\phi}) = \hat{h}(p|\bar{\phi}) - \hat{h}(0|\bar{\phi}) \tag{3-13}$$

Figure III.3.9. shows $\hat{T}(p|\phi)$ for $L = 8$ and for several background fields.

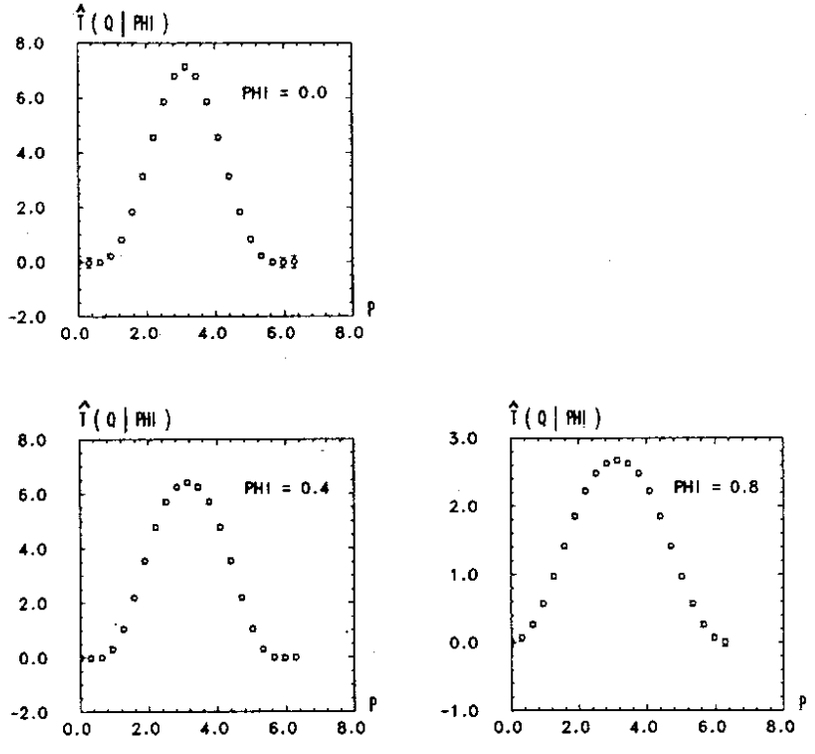

Figure III.3.9. The pictures show the Fourier transform of the kinetic operator T along the diagonal $q = (p, p)$. By definition $\hat{T}(q|\phi) \equiv \sum_x T(0, x|\phi) \cdot \cos qx$. The background fields ϕ are constant, the block size is $L = 8$, the Gaussian parameter $\kappa = 12$. Since Monte Carlo results for $h(0, x|\phi)$ are available only for $|x| \leq 3$ the sum over x was truncated. In order to determine statistical errors the Fourier transformation was done separately on 10 subgroups of the data.

For $\phi = 0.0$ and $\phi = 0.4$ the local stationarity of $\hat{T}$ at $p = 0$ shows that the system here is close to "antiferromagnetic" behaviour.

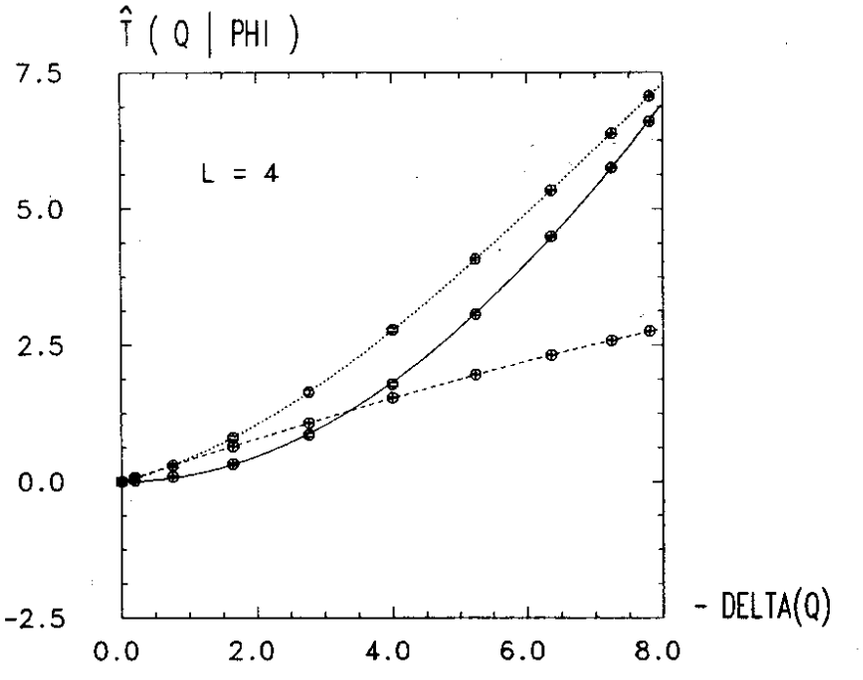

Figure III.3.10. $\hat{T}(q|\phi)$ along the diagonal $q \equiv (p, p)$, plotted vs. the Fourier transform of the Laplacian $-\tilde{\Delta}(q) = 8 \sin^2 \frac{p}{2}$. This representation allows a determination of a least square fit with polynomials in $-\tilde{\Delta}(q)$ in order to determine the coefficients of a series[1]

$$T(0, x|\phi) \approx t_1 \cdot [-\Delta](0, x) + t_2 \cdot [-\Delta]^2(0, x) + t_3 \cdot [-\Delta]^3(0, x)$$

The Gaussian parameter is $\kappa = 12$. The dots with error bars show the Monte Carlo results for $\hat{T}$. The curves show least square fits with cubic polynomials in $-\tilde{\Delta}$.

$\phi = 0.0$: full line

$\phi = 0.4$: dotted line

$\phi = 0.8$: dashed line

Results for the coefficients of the least square fits are displayed in the table next page.

[1] The real space matrix elements of Δ^n for $n \leq 4$ can be found in Appendix C.2.

The following table shows results of least square fits for the determination of coefficients in an approximation of the kinetic operator with powers $T(0,x|\phi)$ of the Laplacian:

$$h(0,x|\phi) = t_1 \cdot [-\Delta](0,x) + t_2 \cdot [-\Delta]^2(0,x) + t_3 \cdot [-\Delta]^3(0,x) \qquad (3\text{-}14)$$

L = 4	t_1	t_2	t_3
$\phi = 0.0$	$-8.6 \cdot 10^{-3}$	$1.2 \cdot 10^{-1}$	$-1.7 \cdot 10^{-3}$
$\phi = 0.2$	$-9.6 \cdot 10^{-2}$	$1.7 \cdot 10^{-1}$	$-5.6 \cdot 10^{-3}$
$\phi = 0.4$	$3.1 \cdot 10^{-1}$	$1.2 \cdot 10^{-1}$	$-5.0 \cdot 10^{-3}$
$\phi = 0.6$	$5.8 \cdot 10^{-1}$	$3.5 \cdot 10^{-2}$	$-2.0 \cdot 10^{-3}$
$\phi = 0.8$	$4.0 \cdot 10^{-1}$	$-1.6 \cdot 10^{-3}$	$-5.1 \cdot 10^{-4}$
$\phi = 1.0$	$1.6 \cdot 10^{-1}$	$1.2 \cdot 10^{-5}$	$-2.6 \cdot 10^{-4}$
$\phi = 1.2$	$9.6 \cdot 10^{-2}$	$-7.2 \cdot 10^{-3}$	$4.4 \cdot 10^{-4}$
$\phi = 1.4$	$4.2 \cdot 10^{-2}$	$-2.7 \cdot 10^{-3}$	$1.5 \cdot 10^{-4}$

L = 8	t_1	t_2	t_3
$\phi = 0.0$	$-9.7 \cdot 10^{-2}$	$1.5 \cdot 10^{-1}$	$-3.5 \cdot 10^{-3}$
$\phi = 0.2$	$-2.6 \cdot 10^{-1}$	$2.5 \cdot 10^{-1}$	$-1.3 \cdot 10^{-2}$
$\phi = 0.4$	$-1.7 \cdot 10^{-1}$	$2.4 \cdot 10^{-1}$	$-1.4 \cdot 10^{-2}$
$\phi = 0.6$	$4.8 \cdot 10^{-1}$	$4.3 \cdot 10^{-2}$	$-2.9 \cdot 10^{-3}$
$\phi = 0.8$	$3.2 \cdot 10^{-1}$	$1.6 \cdot 10^{-2}$	$-1.7 \cdot 10^{-3}$
$\phi = 1.0$	$2.0 \cdot 10^{-1}$	$4.0 \cdot 10^{-3}$	$1.5 \cdot 10^{-5}$
$\phi = 1.2$	$1.1 \cdot 10^{-1}$	$-2.8 \cdot 10^{-3}$	$7.0 \cdot 10^{-6}$
$\phi = 1.4$	$9.0 \cdot 10^{-2}$	$-9.0 \cdot 10^{-3}$	$5.0 \cdot 10^{-4}$

The table clearly shows that for small ϕ the "kinetic coupling" t_1 becomes small or even negative, whereas the parameter t_2 is much larger. t_3 is quite small for any ϕ. The conclusion from this observation is that an approximation of the effective Hamiltonian in the form

$$\mathcal{H}_{\rm eff}(\phi) = \frac{\rho}{2} \sum_x \phi(x)[-\Delta\phi](x) + \sum_x \mathcal{V}_{\rm eff}[\phi(x)] \qquad (3\text{-}15)$$

is impossible. However, in a neighbourhood of $\phi = 1.0$ - the effective potential takes its minimum there - one has a positive kinetic coupling t_1 and small nonlocal corrections which are described by the parameters t_2 and t_3.

Chapter IV

A Monte Carlo Method for the Computation of Taylor Expansions for the Effective Hamiltonian of φ^4 Theory

The method of fixed block spins is easy to apply if the fundamental lattice field variables are free of constraints (as for example $\varphi(x)^2 = 1$ in the $O(N)$ symmetric nonlinear σ-model). An example for a theory without constraints is φ^4 theory.

In spite of the simplicity of its bare Hamiltonian φ^4 theory is of interest. The four-component model is an important ingredient of Glashow-Salam-Weinberg-theory of electroweak interactions. In two and in three dimensions φ^4 theory is superrenormalizable in perturbation theory and a nontrivial continuum limit exists [11 and references cited therein]. φ^4 theory in four dimensions is renormalizable in perturbation theory. Little doubt exists that the modell has a trivial continuum limit, i.e. is not renormalizable beyond perturbation theory: The lattice cutoff can only be removed consistently if simultaneously the renormalized coupling constant goes to zero, see [16] and references cited therein. A careful MCRG study for φ^4 theory is e.g. the paper of Lang [43].

This chapter deals with scalar φ^4 theory. By a suitable transformation of the fundamental variables a generating functional is derived for Taylor coefficients of the effective Hamiltonian $\mathcal{H}_{\rm eff}(\phi)$ (Section IV.1.). The Taylor expansion can be set up about arbitrary reference configurations $\bar{\phi}$. This is achieved by splitting the fundamental field into a fluctuation field and a part determined by the block spin and the background field $\bar{\phi}$. The fluctuation field obeys the constraint that the block averages exactly equal the prescribed background field $\bar{\phi}$. The degrees of freedom parametrized by the fluctuation fields shall be integrated out with the help of the Monte Carlo method.

The operators appearing in the expansion are products of block spin fields. The Taylor kernels can be expressed in terms of truncated correlation function of the fluctuation fields. For suitably chosen background field $\bar{\phi}$ one expects that a Taylor series exists and has good locality properties. The effective Hamiltonian has good locality properites if the (truncated) correlation functions of the fluctuation fields are of short range. However, if $\bar{\phi}$ is a very unlikely block spin configuration one has to be aware of nonlocalities (large field problem, see also Chapter III). The method described in this chapter is well suited to study this problem, in particular for a large value of the bare quartic coupling where analytical methods are not applicable at present.

Two independent methods for the computation of the effective potential $\mathcal{V}_{\rm eff}(\phi)$ are described in Section IV.2. The derivatives of the effective potential can be expressed as sums of truncated correlation functions with constant background field (zero momentum correlation functions). The speed of convergence of these sums is a criterion for locality of the Taylor expansions for $\mathcal{H}_{\rm eff}(\phi)$ about constant reference fields $\bar{\phi}$. The second method for the computation of $\mathcal{V}_{\rm eff}(\phi)$ is based on integration of $(\partial/\partial\phi)\mathcal{V}_{\rm eff}(\phi)$ over ϕ. Since $(\partial/\partial\phi)\mathcal{V}_{\rm eff}(\phi)$ can be directly computed by Monte Carlo simulations with constant background fields ϕ the effective potential can be computed this way. From fits with polynomials or splines one then can determine the derivatives of $\mathcal{V}_{\rm eff}(\phi)$.

From the Monte Carlo data for the 2-point Taylor kernels for $\mathcal{H}_{\rm eff}(\phi)$ one can extract an effective kinetic term. This in particular allows to define a wave function renormalization. If the wave function renormalization has been determined, the renormalized mass and the renormalized ϕ^4 coupling can be computed from the effective potential.

Section IV.3. contains the essential technical details for a realization of the Monte Carlo procedure.

This chapter is organized as follows:

IV.1. *Generating Functional for the Taylor Coefficients of $\mathcal{H}_{\rm eff}(\phi)$*

IV.2. *Effective Potential and Effective Kinetic Term*

IV.3. *Details of the Monte Carlo Procedure*

IV.1. Generating Functional for the Taylor Coefficients of $\mathcal{H}_{\rm eff}(\phi)$

By a shift in the fundamental variables a generating functional is derived for coefficients of a Taylor expansion for $\mathcal{H}_{\rm eff}(\phi)$ about arbitrary block spin configurations $\bar{\phi}$.

We consider scalar φ^4 theory on a cubic d-dimensional lattice Λ with periodic boundary conditions.

$$Z = \int \prod_{z\in\Lambda} d\varphi(z)\, e^{-\mathcal{H}(\varphi)} \tag{1-1}$$

Since we use *lattice units* the field variables φ (spins) will be dimensionless quantities. $\mathcal{H}(\varphi)$ is the Hamiltonian

$$\mathcal{H}(\varphi) = \frac{1}{2}\sum_{z\in\Lambda}\varphi(z)[-\Delta\varphi](z) + \frac{m_0^2}{2}\sum_{z\in\Lambda}\varphi(z)^2 + \frac{\lambda_0}{4!}\sum_{z\in\Lambda}\varphi(z)^4 \tag{1-2}$$

m_0^2 and λ_0 denote the bare mass squared and quartic coupling constant, respectively. We have

$$\frac{1}{2}\sum_{z\in\Lambda}\varphi(z)[-\Delta\varphi](z) = \frac{1}{2}\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\varphi(z+\hat{\mu})-\varphi(z)]^2 \tag{1-3}$$

An effective Hamiltonian $\mathcal{H}_{\rm eff}(\phi)$ for (dimensionless) block spins ϕ on the block lattice Λ' is defined through the effective Boltzmannian

$$e^{-\mathcal{H}_{\rm eff}(\phi)} \equiv \int \prod_{z\in\Lambda} d\varphi(z) \prod_{z\in\Lambda'} \delta[\phi(x) - L^{\frac{1}{2}(d-2+\eta)} \operatorname*{av}_{z\in x}\varphi(z)]\, e^{-\mathcal{H}(\varphi)} \equiv \mathcal{Z}(\phi) \tag{1-4}$$

In the neighbourhood of a renormalization group fixed point η has the meaning of a critical exponent (anomalous dimension, see Chapter I). The wave function renormalization will be

fixed by a renormalization condition, e.g. the condition that the coupling constant for the kinetic term equals $\frac{1}{2}$.

After the dilatations $\phi \to L^{\eta/2}\phi$ and $\varphi \to L^{-\frac{1}{2}(d-2)}\varphi$ the scale factors are removed from the δ-function:

$$e^{-\mathcal{H}_{\rm eff}(L^{\eta/2}\phi)} = \int \prod_{z\in\Lambda} d\varphi(z) \prod_{z\in\Lambda'} \delta[\phi(x) - \operatorname*{av}_{z\in x}\varphi(z)]\, e^{-\mathcal{H}(L^{-\frac{1}{2}(d-2)}\varphi)} = \mathcal{Z}(L^{\eta/2}\phi) \tag{1-5}$$

We want to derive a Taylor expansion for $\mathcal{H}_{\rm eff}(\phi)$. The Taylor kernels will be obtained by differentiating with respect to the block spins $\phi(x)$. In order to render possible "unconstrained" differentiation we will remove the ϕ-dependence from the δ-function. The Taylor expansion shall be about a reference configuration $\bar{\phi}$. Thus the variables will be fields $\psi(x) \equiv \phi(x) - \bar{\phi}(x)$. We write

$$\begin{aligned} \varphi(z) &= \check{\psi}(z) + \zeta(z) \\ \check{\psi}(z) &\equiv \psi(x) \quad \text{for } z \in x \end{aligned} \tag{1-6}$$

$\check{\psi}$ is determined by the block spin field ϕ and the back ground field $\bar{\phi}$. ζ is called fluctuation field. The degrees of freedom parametrized by ζ have to be integrated out in order to determine the effective theory:

$$e^{-\tilde{\mathcal{H}}_{\rm eff}(\phi)} \equiv \int \prod_{z\in\Lambda} d\zeta(z) \prod_{z\in\Lambda'} \delta[\bar{\phi}(x) - \operatorname*{av}_{z\in x}\zeta(z)]\, e^{-\tilde{\mathcal{H}}(\check{\psi}+\zeta)} \equiv \tilde{\mathcal{Z}}(\phi) \tag{1-7}$$

Rescaled quantities have been introduced:

$$\begin{aligned} \tilde{\mathcal{H}}(\varphi) &\equiv \mathcal{H}(L^{-\frac{1}{2}(d-2)}\varphi) \\ \tilde{\mathcal{H}}_{\rm eff}(\phi) &\equiv \mathcal{H}_{\rm eff}(L^{\frac{\eta}{2}}\phi) \\ \tilde{\mathcal{Z}}(\phi) &\equiv \mathcal{Z}(L^{\frac{\eta}{2}}\phi) \end{aligned} \tag{1-8}$$

For φ^4 theory rescaling of the fields is equivalent to a change in the bare coupling constants:

$$\begin{aligned} \tilde{\mathcal{H}}(\varphi) &= \mathcal{H}(L^{-\frac{1}{2}(d-2)}\varphi) \\ &= \frac{\tilde{\kappa}_0}{2}\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\varphi(z+\hat{\mu})-\varphi(z)]^2 + \frac{\tilde{m}_0^2}{2}\sum_{z\in\Lambda}\varphi(z)^2 + \frac{\tilde{\lambda}_0}{4!}\sum_{z\in\Lambda}\varphi(z)^4 \end{aligned} \tag{1-9}$$

The "rescaled" coupling constants $\tilde{\kappa}_0$, $\tilde{m}_0^2$ and $\tilde{\lambda}_0$ are given by

$$\begin{aligned}\tilde{\kappa}_0 &= L^{-(d-2)} \\ \tilde{m}_0^2 &= L^{-(d-2)} m_0^2 \\ \tilde{\lambda}_0 &= L^{-2(d-2)} \lambda_0\end{aligned} \tag{1-10}$$

We now write $\tilde{\mathcal{H}}(\tilde{\psi} + \zeta)$ as a sum of three contributions:

$$\tilde{\mathcal{H}}(\tilde{\psi} + \zeta) = \tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi}) + \tilde{\mathcal{H}}(\zeta) + R(\psi|\zeta) \tag{1-11}$$

$\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi})$ is a trivial term which does not depend on the fluctuation field. The coupling of the fluctuation field to the block spin is described by $R(\psi|\zeta)$. This split is done explicitly in Appendix C.1. For $\psi = 0$ the sum $\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi}) + R(\psi|\zeta)$ vanishes. Therefore the following equation holds:

$$\frac{\tilde{\mathcal{Z}}(\phi)}{\tilde{\mathcal{Z}}(\bar{\phi})} = e^{-\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi})} \cdot \langle e^{-R(\psi|\zeta)} \rangle_{\bar{\phi}} \tag{1-12}$$

The $\bar{\phi}$-parametric expectation value is defined as follows

$$\langle \mathcal{O}(\zeta) \rangle_{\bar{\phi}} \equiv \tilde{\mathcal{Z}}(\bar{\phi})^{-1} \cdot \int \prod_{z \in \Lambda} d\zeta(z) \prod_{x \in \Lambda'} \delta[\bar{\phi}(x) - \operatorname*{av}_{z \in x} \zeta(z)]\, e^{-\tilde{\mathcal{H}}(\zeta)}\, \mathcal{O}(\zeta) \tag{1-13}$$

For the effective Hamiltonian one obtains the expression

$$\tilde{\mathcal{H}}_{\text{eff}}(\phi) - \tilde{\mathcal{H}}_{\text{eff}}(\bar{\phi}) = \tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi}) - \ln \langle e^{-R(\psi|\zeta)} \rangle_{\bar{\phi}} \tag{1-14}$$

A Taylor expansion for $\tilde{\mathcal{H}}_{\text{eff}}(\phi)$ about $\phi = \bar{\phi}$ corresponds to an expansion about $\psi = 0$. For the coefficients $\tilde{h}$ in the series

$$\tilde{\mathcal{H}}_{\text{eff}}(\phi) = \tilde{\mathcal{H}}_{\text{eff}}(\bar{\phi}) + \sum_{n \geq 1} \frac{1}{n!} \sum_{x_1 \in \Lambda'} \cdots \sum_{x_n \in \Lambda'} \tilde{h}(x_1 \dots x_n|\bar{\phi}) \cdot \psi(x_1) \dots \psi(x_n) \tag{1-15}$$

we find

$$\tilde{h}(x_1 \dots x_n|\bar{\phi}) = \frac{\delta}{\delta\psi(x_1)} \cdots \frac{\delta}{\delta\psi(x_n)} \cdot \left[\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi}) - \ln \langle e^{-R(\psi|\zeta)} \rangle_{\bar{\phi}}\right]\Big|_{\psi=0} \tag{1-16}$$

For φ^4 theory (see Appendix C.1.)

$$\begin{aligned}\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi}) = \sum_{x \in \Lambda'} \Big\{ &\frac{L}{2} \sum_{\mu=1}^{d} [\psi(x + \hat{\mu}') - \psi(x)]^2 \\ &+ \frac{L^2 m_0^2}{2} [\psi(x)^2 + 2\bar{\phi}(x)\psi(x)] \\ &+ \frac{L^{4-d}\lambda_0}{4!} [\psi(x)^4 + 4\bar{\phi}(x)\psi(x)^3] \Big\}\end{aligned} \tag{1-17}$$

The term coupling the fluctuation field ζ to ψ is quadratic in ψ:

$$R(\psi|\zeta) = \sum_{x \in \Lambda'} \psi(x) \cdot \Xi_1(x|\zeta) + \sum_{x \in \Lambda'} \psi(x)^2 \cdot \Xi_2(x|\zeta) \tag{1-18}$$

$\Xi_1(x|\zeta)$ and $\Xi_2(x|\zeta)$ are given by

$$\begin{aligned}\Xi_1(x|\zeta) &= \frac{L^{4-d}\lambda_0}{6} \operatorname*{av}_{z \in x} \zeta(z)^3 + L^2 \operatorname*{av}_{z \in x} (-\Delta\zeta)(z) \\ \Xi_2(x|\zeta) &= \frac{L^{4-d}\lambda_0}{4} \operatorname*{av}_{z \in x} \zeta(z)^2\end{aligned} \tag{1-19}$$

If one differentiates at most once with respect to each $\psi(x)$ the quadratic term in $R(\psi|\zeta)$ can be ignored. For $x_i \neq x_j$, $i, j \leq n$

$$\frac{\delta}{\delta\psi(x_1)} \cdots \frac{\delta}{\delta\psi(x_n)} \cdot \ln \langle e^{-R(\psi|\zeta)} \rangle_{\bar{\phi}}\Big|_{\psi=0} = (-1)^n \langle \Xi_1(x_1|\zeta) \dots \Xi_1(x_n|\zeta) \rangle_{\bar{\phi}}^T \tag{1-20}$$

Let us summarize: The Taylor expansion of $\mathcal{H}_{\text{eff}}(\phi)$ about $\phi = \bar{\phi}$ is given by Eqs. (1-15) ... (1-19). If all arguments $x_1 \dots x_n$ of h are different one can use Eq. (1-20).

IV.2. Effective Potential and Effective Kinetic Term

In this section two independent methods are described to compute the effective potential $\mathcal{V}_{\text{eff}}(\phi)$. It is shown how one can obtain an effective kinetic term from the quadratic Taylor coefficients.

Let us recall the definition of the effective potential:

$$\mathcal{V}_{\text{eff}}(\phi) = \mathcal{H}_{\text{eff}}(\phi)\big|_{\phi=\text{const}} / |\Lambda'| \tag{2-1}$$

It follows from Eq. (1-14) that

$$\tilde{\mathcal{V}}_{\text{eff}}(\phi) - \tilde{\mathcal{V}}_{\text{eff}}(\bar{\phi}) = \tilde{\mathcal{W}}_{\text{eff}}(\psi|\bar{\phi}) - |\Lambda'|^{-1} \ln \langle e^{-R(\psi=\text{const}|\zeta)} \rangle_{\bar{\phi}=\text{const}} \tag{2-2}$$

$\tilde{\mathcal{W}}_{\text{eff}}(\psi|\bar{\phi})$ equals $\tilde{\mathcal{T}}_{\text{eff}}(\psi|\bar{\phi})$ per volume for constant fields ψ and $\bar{\phi}$:

$$\tilde{\mathcal{W}}_{\text{eff}}(\psi|\bar{\phi}) = \frac{L^2 m_0^2}{2}\left[\psi^2 + 2\bar{\phi}\psi\right] + \frac{L^{4-d}\lambda_0}{4!}\left[\psi^4 + 4\bar{\phi}\psi^3\right] \tag{2-3}$$

For constant ψ the exponent R is simplified considerably:

$$R(\psi|\zeta) = \psi \cdot A(\zeta) + \psi^2 \cdot B(\zeta)$$

$$\begin{aligned} A(\zeta) &= \frac{1}{6} L^{4-d}\lambda_0 \cdot \operatorname*{av}_{z\in\Lambda} \zeta(z)^3 \\ B(\zeta) &= \frac{1}{4} L^{4-d}\lambda_0 \cdot \operatorname*{av}_{z\in\Lambda} \zeta(z)^2 \end{aligned} \tag{2-4}$$

The contribution with $(-\Delta\zeta)$ no longer occurs because for periodic boundary conditions the sum $\sum_{z\in\Lambda}(-\Delta\zeta)(z)$ vanishes for all configurations ζ.

We now consider a Taylor expansion for the effective potential in powers of ψ:

$$\tilde{\mathcal{V}}_{\text{eff}}(\phi) - \tilde{\mathcal{V}}_{\text{eff}}(\bar{\phi}) = \sum_{n\geq 1} \frac{\tilde{\mathcal{V}}^{(n)}_{\text{eff}}(\bar{\phi})}{n!} \cdot \psi^n \tag{2-5}$$

$$\tilde{\mathcal{V}}^{(n)}_{\text{eff}}(\bar{\phi}) = \left(\frac{d}{d\psi}\right)^n \left[\tilde{\mathcal{W}}_{\text{eff}}(\psi|\bar{\phi}) - |\Lambda'|^{-1} \ln \langle e^{-R(\psi|\zeta)}\rangle_{\bar{\phi}}\right]\Big|_{\psi=0} \tag{2-6}$$

The expansion coefficients for $\tilde{\mathcal{W}}_{\text{eff}}(\psi|\bar{\phi})$ can be read off directly from Eq. (2-3):

$$\begin{aligned} \tilde{\mathcal{W}}^{(1)}_{\text{eff}}(\bar{\phi}) &= L^2 m_0^2 \cdot \bar{\phi} \\ \tilde{\mathcal{W}}^{(2)}_{\text{eff}}(\bar{\phi}) &= L^2 m_0^2 \\ \tilde{\mathcal{W}}^{(3)}_{\text{eff}}(\bar{\phi}) &= L^{4-d}\lambda_0 \cdot \bar{\phi} \\ \tilde{\mathcal{W}}^{(4)}_{\text{eff}}(\bar{\phi}) &= L^{4-d}\lambda_0 \end{aligned} \tag{2-7}$$

The following table shows the coefficients $\tilde{\mathcal{V}}^{(n)}_{\text{eff}}(\bar{\phi})$ for $n \leq 4$, expressed in terms of truncated correlation functions of observables $A(\zeta)$ and $B(\zeta)$.

$$\begin{aligned} \tilde{\mathcal{V}}^{(1)}_{\text{eff}}(\bar{\phi}) &= L^2 m_0^2 \cdot \bar{\phi} + |\Lambda'|^{-1}\langle A\rangle_{\bar{\phi}} \\ \tilde{\mathcal{V}}^{(2)}_{\text{eff}}(\bar{\phi}) &= L^2 m_0^2 + |\Lambda'|^{-1}\left\{-\langle A^2\rangle^T_{\bar{\phi}} + 2\langle B\rangle_{\bar{\phi}}\right\} \\ \tilde{\mathcal{V}}^{(3)}_{\text{eff}}(\bar{\phi}) &= L^{4-d}\lambda_0 \cdot \bar{\phi} + |\Lambda'|^{-1}\left\{\langle A^3\rangle^T_{\bar{\phi}} - 6\langle AB\rangle^T_{\bar{\phi}}\right\} \\ \tilde{\mathcal{V}}^{(4)}_{\text{eff}}(\bar{\phi}) &= L^{4-d}\lambda_0 + |\Lambda'|^{-1}\left\{-\langle A^4\rangle^T_{\bar{\phi}} + 12\langle A^2 B\rangle^T_{\bar{\phi}} - 12\langle B^2\rangle^T_{\bar{\phi}}\right\} \end{aligned} \tag{2-8}$$

For $\bar{\phi} = 0$ the expectation values of observables which are even in ζ vanish. In particular, only the $\tilde{\mathcal{V}}^{(n)}_{\text{eff}}$ with even n do not vanish. As an example let us consider the renormalized mass squared $\tilde{m}_R^2 \equiv \tilde{\mathcal{V}}^{(2)}_{\text{eff}}(0)$. With

$$\begin{aligned} A_x(\zeta) &\equiv L^{4-d}\frac{\lambda_0}{6} \operatorname*{av}_{z\in x} \zeta^3 \\ B_x(\zeta) &\equiv L^{4-d}\frac{\lambda_0}{4} \operatorname*{av}_{z\in x} \zeta^2 \end{aligned} \tag{2-9}$$

because of translational invariance for constant $\bar{\phi}$

$$\begin{aligned} \langle A(\zeta)^2\rangle_{\bar{\phi}} &= |\Lambda'| \cdot \sum_{x\in\Lambda'} \langle A_0(\zeta) A_x(\zeta)\rangle_{\bar{\phi}} \\ \langle B(\zeta)\rangle_{\bar{\phi}} &= |\Lambda'| \cdot \langle B_x(\zeta)\rangle_{\bar{\phi}} \end{aligned} \tag{2-10}$$

If for a given $\bar{\phi}$ the correlations $\langle A_0(\zeta)A_x(\zeta)\rangle_{\bar{\phi}}$ are of short range the sum on the right hand side of Eq. (2-10) will converge rapidly. This can be and should be investigated for several $\bar{\phi}$ with the Monte Carlo method described in this chapter.

The second possibility to determine $\tilde{\mathcal{V}}_{\text{eff}}(\phi)$ is to integrate $\tilde{\mathcal{V}}^{(1)}_{\text{eff}}(\bar{\phi})$ over $\bar{\phi}$. We have

$$\tilde{\mathcal{V}}_{\text{eff}}(\phi) = \frac{L^2 m_0^2}{2}\phi^2 + \int_0^\phi d\bar{\phi}\,\langle A_x(\zeta)\rangle_{\bar{\phi}} \tag{2-11}$$

The integration constant has been chosen such that $\tilde{\mathcal{V}}_{\text{eff}}(0) = 0$.

In order to perform the integral over $\bar{\phi}$ one will compute $\langle A_x(\zeta)\rangle_{\bar{\phi}} = \frac{1}{6}L^{4-d}\lambda_0\langle \text{av}_{z\in x}\,\zeta(z)^3\rangle_{\bar{\phi}}$ for a set of $\bar{\phi}$-values (e.g $\bar{\phi} = 0.0, 0.1, \ldots, 1.5$) with the Monte Carlo method and than interpolate or fit the measured data. One might use splines. A fit with polynomials might also be useful because this would allow to directly read off the renormalized coupling constants.

For the following we will assume that the effective Hamiltonian $\mathcal{H}_{\text{eff}}(\phi)$ can be expanded about $\phi = 0$. This will at least be possible if the effective potential takes its absolute minimum at $\phi = 0$.

It will be shown in Appendix C.2. how translational invariant Taylor kernels $\tilde{h}(x, y|\bar{\phi})$ can be expanded in "powers of the Laplacian":

$$\tilde{h}(0, x|\bar{\phi}) = \tilde{\mathcal{V}}''_{\text{eff}}(\bar{\phi}) + \tilde{\kappa}_R(\bar{\phi})[-\Delta(0, x)] + \ldots \tag{2-12}$$

$\tilde{\mathcal{V}}''_{\text{eff}}(\bar{\phi}) = \sum_x \tilde{h}(0, x|\bar{\phi})$ is the second derivative of the effective potential. $\tilde{\kappa}_R \equiv \tilde{\kappa}_R(\bar{\phi} = 0)$ denotes the kinetic coupling in an expansion

$$\tilde{\mathcal{H}}_{\text{eff}}(\phi) = \frac{\tilde{\kappa}_R}{2}\sum_x \phi(x)[-\Delta\phi](x) + \sum_x \tilde{\mathcal{V}}_{\text{eff}}[\phi(x)] + \ldots \tag{2-13}$$

According to Appendix C.2.

$$\tilde{\kappa}_R = -\frac{1}{2d}\sum_x \tilde{h}(0,x|\bar{\phi}=0)\cdot x^2 \tag{2-14}$$

Taking into account the contribution from $\tilde{\tau}_{\rm eff}(\phi|\bar{\phi}=0)$ one finds

$$\tilde{\kappa}_R = L + \frac{1}{2d}\sum_x \langle \Xi_1(0|\zeta)\cdot\Xi_1(x|\zeta)\rangle^T_{\bar{\varphi}=0}\cdot x^2 \tag{2-15}$$

IV.3. Details of the Monte Carlo Procedure

An updating procedure for the fluctuation field ζ is described. The constraint that the block averages must not be changed is taken into account by an algorithm which simultaneously updates randomly chosen pairs of spins belonging to the same block.

In order to compute Taylor coefficients of the effective Hamiltonian we want to evaluate expectation values $\langle(\cdot)\rangle_{\bar{\phi}}$ with the help of the Monte Carlo method. The computer has to generate ζ-configurations which are distributed statistically with a probability density

$$\mathrm{dprob}(\zeta) \propto \prod_{z\in\Lambda} d\zeta(z) \prod_{x\in\Lambda'} \delta[\bar{\phi}(x) - \underset{z\in x}{\mathrm{av}}\,\zeta(z)]e^{-\tilde{\mathcal{H}}(\zeta)} \tag{3-1}$$

The rescaled fundamental Hamiltonian $\tilde{\mathcal{H}}(\zeta)$ was defined by

$$\tilde{\mathcal{H}}(\zeta) = \frac{\tilde{\kappa}_0}{2}\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\zeta(z+\hat{\mu})-\zeta(z)]^2 + \frac{\tilde{m}_0^2}{2}\sum_{z\in\Lambda}\zeta(z)^2 + \frac{\tilde{\lambda}_0}{4!}\sum_{z\in\Lambda}\zeta(z)^4 \tag{3-2}$$

For the purpose of Monte Carlo calculations it is useful to rearrange the Hamiltonian a little bit. Since

$$\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\zeta(z+\hat{\mu})-\zeta(z)]^2 = -2\sum_{z\in\Lambda}\sum_{\mu=1}^{d}\zeta(z)\zeta(z+\hat{\mu}) + 2d\sum_{z\in\Lambda}\zeta(z)^2 \tag{3-3}$$

we have

$$\tilde{\mathcal{H}}(\zeta) = -\tilde{\kappa}_0\sum_{z\in\Lambda}\sum_{\mu=1}^{d}\zeta(z)\zeta(z+\hat{\mu}) + \tilde{\rho}_0\sum_{z\in\Lambda}\zeta(z)^2 + \frac{\tilde{\lambda}_0}{4!}\sum_{z\in\Lambda}\zeta(z)^4 \tag{3-4}$$

The coupling $\tilde{\rho}_0$ is given by

$$\tilde{\rho}_0 \equiv \frac{1}{2}(\tilde{m}_0^2 + 2d\tilde{\kappa}_0) \tag{3-5}$$

The measure defined by Eq. (3-1) does not allow to change a single variable $\zeta(z)$. This would contradict the condition that the block average is fixed to the value of the background field $\bar{\varphi}$. The most simple solution for this problem is to update two variables simultaneously. We consider pairs $\{\zeta_1 \equiv \zeta(z_1), \zeta_2 \equiv \zeta(z_2)\}$ with z_1, z_2 belonging to the same block x. The conditional probability distribution for the pair $\{\zeta_1,\zeta_2\}$ is given by

$$\mathrm{dprob}(\zeta_1,\zeta_2) \propto d\zeta_1 d\zeta_2\cdot\delta[\zeta_1+\zeta_2-\zeta_{12}]\cdot e^{\tilde{\kappa}_0[t_1\zeta_1+t_2\zeta_2+\epsilon\zeta_1\zeta_2]-\tilde{\rho}_0[\zeta_1^2+\zeta_2^2]-\frac{\tilde{\lambda}_0}{4!}[\zeta_1^4+\zeta_2^4]} \tag{3-6}$$

The ϵ-parameter takes care of the special case that z_1 and z_2 are nearest neighbours:

$$\epsilon \equiv \begin{cases} 1 & \text{if} \quad z_1, z_2 \quad \text{nearest neighbours} \\ 0 & \text{else} \end{cases} \tag{3-7}$$

Further definitions are

$$\begin{aligned} t_1 &\equiv \sum_{<z,z_1>}\zeta(z) - \epsilon\zeta_2 \\ t_2 &\equiv \sum_{<z,z_2>}\zeta(z) - \epsilon\zeta_1 \end{aligned} \tag{3-8}$$

The sum $\sum_{<z,z_i>}$ runs over the 2d nearest neighbours of z_i. One should recognize that t_1 and t_2 do not depend on ζ_1 and ζ_2. ζ_{12} is the sum of ζ_1 and ζ_2 before the updating, $\zeta_{12} = \zeta_1^{\rm old} + \zeta_2^{\rm old}$. After the linear and nonsingular variable transformation

$$\begin{aligned} \zeta_1 &\equiv \zeta_+ + \zeta_- \\ \zeta_2 &\equiv \zeta_+ - \zeta_- \end{aligned} \tag{3-9}$$

it is obvious that $\zeta_+ = \frac{1}{2}(\zeta_1+\zeta_2)$ must not be changed. The conditional probability distribution for $\zeta_- = \frac{1}{2}(\zeta_1-\zeta_2)$ is given by

$$\begin{aligned} \mathrm{dprob}(\zeta_-) &\propto d\zeta_-\cdot e^{\tilde{\kappa}_0[(t_1-t_2)\zeta_- - \epsilon\zeta_-^2] - \tilde{\rho}_0[2\zeta_-^2] - \tilde{\lambda}_0[12\zeta_+^2\zeta_-^2 + 2\zeta_-^4]} \\ &\propto d\zeta_-\cdot e^{K_1\zeta_- - K_2\zeta_-^2 - K_4\zeta_-^4} \end{aligned} \tag{3-10}$$

with couplings

$$\begin{aligned} K_1 &= \tilde{\kappa}_0(t_1-t_2) \\ K_2 &= 2\tilde{\rho}_0 + \epsilon\tilde{\kappa}_0 + \frac{\tilde{\lambda}_0}{2}\zeta_+^2 \\ K_4 &= \frac{\tilde{\lambda}_0}{12} \end{aligned} \tag{3-11}$$

There are several possibilities to generate random numbers ζ_- which are distributed according to Eq. (3-10). As an example an algorithm is described which is applicable if $K_2 > 0$. The couplings K_1 and K_2 depend on the actual ζ-configuration. However, $K_2 \geq 2\tilde{\rho}_0$. Furthermore, $\tilde{\rho}_0$ is positive if $m_0^2 + 2d > 0$. This will be assumed in the following. Eq. (3-10) can be written as

$$\mathrm{dprob}(\zeta_-) \propto d\mu_{a,b}(\zeta_-) \cdot e^{-K_4 \zeta_-^4} \tag{3-12}$$

with the Gaussian measure

$$\begin{aligned} d\mu_{a,b}(\zeta_-) &\propto d\zeta_- \cdot e^{-(\zeta_- - a)^2/(2b^2)} \\ a &= K_1/(2K_2) \\ b &= 1/\sqrt{2K_2} \end{aligned} \tag{3-13}$$

Gaussian random number according to $d\mu_{a,b}$ can for example be generated with the help of the NAGLIB-routine G05DDE [48]. The quartic coupling K_4 will then be taken into account by a "Metropolis filter": A candidate ζ_-^{new} generated according to $d\mu_{a,b}(\zeta_-^{\mathrm{new}})$ will be accepted with "probability"

$$\omega \equiv e^{-K_4[(\zeta_-^{\mathrm{new}})^4 - (\zeta_-^{\mathrm{old}})^4]} \tag{3-14}$$

A complete sweep through the ζ-lattice can be done as follows: One sweeps through the lattice, either regularly or randomly. At $z_1 \in x$ one randomly selects an updating partner z_2, with uniform probability over block x. A new ζ_- is generated (e.g. as described above). ζ_1 and ζ_2 are updated accordingly. Then one proceeds to the next site z_1. This procedure is ergodic. It is not necessary to use randomly selected pairs of variables. However, experience with spin models (Chapter II) indicates that this improves the diffusion of information over the blocks. This will have a positive effect on the performance of the Monte Carlo simulation (equilibration, sweep to sweep correlations, critical slowing down).

Summary and Outlook

In this paper it was shown that it is possible to compute effective Hamiltonians for critical or nearly critical lattice field theories without simulating the full (critical or nearly critical) theory. This is in the spirit of the central idea of Wilson's renormalization group philosophy. Monte Carlo calculations performed for the Ising model and the O(3) symmetric nonlinear σ-model on 2-dimensional lattices prove the practicability of the method and yield impressive results.

The procedure described in Chapter II ("Integration over β") allowed a study of the renormalization group flow of the effective potential for 2-dimensional spin models with block spins of fluctuating length. A Monte Carlo algorithm which simultaneously updates randomly selected pairs of spins belonging to the same block works well. Simulations of the O(3) model with fixed (constant) block spin fields did not suffer from critical slowing down even for very large values of the inverse temperature β. However, for the Ising model in the neighbourhood of the critical point we found evidence for long range correlations in the auxiliary system if the (constant) block spin was close to $\phi = 0$. This was a first hint to a large field problem. Comparison of the Monte Carlo data with $O(\beta^2)$ Mayer expansions for the effective potential revealed the remarkable quality of the high temperature approximation, especially for the O(3) model.

In Chapter III it was shown that in the case of a Gaussian block spin definition, coefficients of a Taylor expansion for the effective Hamiltonian can be expressed as truncated correlation functions in the auxiliary statistical mechanical system with fixed block spins. Monte Carlo simulations of this auxiliary system are very easy to perform since a single spin updating is possible. The method was used for a renormalization group study of the critical 2-dimensional Ising model. In addition to the effective potential quadratic Taylor coefficients for several constant background fields were computed. It turned out that a Taylor expansion of $\mathcal{H}_{\mathrm{eff}}(\phi)$ about $\phi = 0$ becomes very nonlocal when the UV-cutoff is lowered.

Chapter IV was devoted to φ^4 theory. It was shown that for such a model the computation of coefficients of a Taylor expansion for the effective Hamiltonian is possible also for a δ block spin definition. The Taylor coefficients can be expressed in terms of truncated correlation functions in an auxiliary system with strictly fixed block averages. The Monte Carlo algorithm for the simulation of this auxiliary system was again based on a simultaneous updating of pairs of spins belonging to the same block.

There are many open questions and problems which might be investigated using the Monte Carlo methods described in this paper. For example, 4-dimensional φ^4 theory has been investigated very carefully analytically and numerically. However, it would be interesting to apply the procedure described in Chapter IV to study locality properties of the effective Hamiltonian at large quartic coupling constant. In the limit $\lambda_0 \to \infty$ φ^4 theory becomes the Ising model. One will therefore take advantage of the experience gained studying the 2-dimensional Ising model. An application of the method to lattice gauge theory is also promising. A linear block spin here leads to an effective theory which is called "dielectric lattice gauge theory" [10]. A Gaussian block spin definition is favourable [12] since pairwise updating of gauge variables is a very complicated matter [13].

Analytical renormalization group studies for weakly coupled theories show that one cannot expect analyticity of the effective Hamiltonian in the large field region. In rigorous

renormalization group calculations one therefore does not parametrize the effective theory in the large field region by a Hamiltonian but works with convergent polymer expansions for the effective Boltzmannian. This possibility has not been considered yet in the framework of numerical renormalization group studies. However, the results of this paper show that one has to deal with a large field problem. It is therefore profitable to learn from analytical renormalization group studies and study the possibility to parametrize the effective theory in the large field region by expansions of the effective Boltzmannian.

In this paper we used linear block spin transformations. Integrating out the lengths one can "return" to variables of the fundamental type.[1] It is an interesting question in the context of ferromagnets whether the large field problem for small block spins leads to nonlocalities of the resulting effective Hamiltonian when the lengths are integrated out.

It is an important question for the numerical approach to quantum field theory whether it is possible to find approximate effective Hamiltonians for physically relevant models (like lattice gauge theories) which are sufficiently local to allow for economical computer simulations but which are precise enough to reproduce the long distance behaviour correctly. In this paper a method for the computation of effective Hamiltonians was proposed and investigated which might be useful when studying this question.

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[1] This is also possible with a procedure which keeps block spins fixed.

Appendix A: Supplement to Chapter II

In analytical renormalization group studies Mayer expansions (high temperature expansions) play an important role [9]. Göpfert and Mack successfully used iterated Mayer expansions for a rigorous analysis of the 3-dimensional U(1) lattice gauge theory [8]. A direct high temperature expansion for the effective Hamiltonian is technically more difficult than an expansion in the fundamental theory. This is due to the fact that the notion of connectivity for the Mayer graphs is more complicated: lattice graphs which are not connected in the fundamental lattice interact if they have sites in a common block. However, good reasons exist that even low order Mayer expansions for the effective Hamiltonian might be good approximations. Following Wilson's renormalization group philosophy one expects that the fluctuation integral which determines the effective theory is dominated by short wave fluctuations. But this is the situation where Mayer expansions (= systematic expansions in terms of properties of subsystems of increasing size) are successful. A comparison of Mayer expansions for the effective potential of the O(N) model and the Ising model with Monte Carlo results (see Chapter II) shows that already $O(\beta^2)$ expansions are very good approximations if the blocks are not too large.

A.1. MAYER EXPANSION FOR THE EFFECTIVE POTENTIAL OF THE 2-DIMENSIONAL ISING MODEL

The Mayer expansion is studied for the effective potential of the 2-dimensional Ising model. The expansion is based on the method of "Möbius inversion". The activities of the Mayer graphs which determine the Möbius amplitudes are polynomials in the block spin ϕ and can be given by explicit formulae. The Möbius amplitudes are determined for all graphs X with number of links $|X| \leq 2$. By expansion of the Möbius amplitudes in powers of β a high temperature expansion for the effective potential is derived to second order in β.

The partition function of the Ising model with nearest neighbour interaction on a 2-dimensional cubic lattice Λ is

$$Z = \sum_s e^{-\beta \mathcal{H}(s)}$$
$$\mathcal{H}(s) = -\sum_{z \in \Lambda} \sum_{\mu=1}^{2} s(z) s(z + \hat{\mu}) \tag{1-1}$$

A probability distribution for block spins of fluctuating length ϕ on the block lattice Λ' is given by the effective Boltzmannian

$$e^{-\mathcal{H}_{\rm eff}(\phi)} = \sum_s e^{-\beta\mathcal{H}(s)} \prod_{x\in\Lambda'} \delta[L^2\phi - \sum_{z\in x} s(z)] \equiv \mathcal{Z}(\phi) \tag{1-2}$$

We want to derive an expansion of $\mathcal{H}_{\rm eff}(\phi)$ for small β (high temperature expansion). Let us define $\mathcal{H}^{(0)}_{\rm eff}(\phi) \equiv \mathcal{H}_{\rm eff}(\phi)|_{\beta=0}$. Then

$$e^{-[\mathcal{H}_{\rm eff}(\phi)-\mathcal{H}^{(0)}_{\rm eff}(\phi)]} = \langle e^{-\beta\mathcal{H}(s)}\rangle_{\phi,\beta=0} \equiv \frac{\mathcal{Z}(\phi)}{\mathcal{Z}_0(\phi)} \tag{1-3}$$

The expectation values $\langle\mathcal{O}(s)\rangle_{\phi,\beta=0}$ are averages over all configurations s which are consistent with the prescribed block spin ϕ:

$$\langle\mathcal{O}(s)\rangle_{\phi,\beta=0} = \mathcal{Z}_0(\phi)^{-1} \sum_s \mathcal{O}(s) \prod_{x\in\Lambda'} \delta[L^2\phi(x) - \sum_{z\in x} s(z)] \tag{1-4}$$

The logarithm of Eq. (1-3) gives an expression for $\mathcal{H}_{\rm eff}(\phi)$:

$$\mathcal{H}_{\rm eff}(\phi) = \mathcal{H}^{(0)}_{\rm eff}(\phi) - \ln\langle e^{-\beta\mathcal{H}(s)}\rangle_{\phi,\beta=0} \tag{1-5}$$

Let us first consider $\mathcal{H}^{(0)}_{\rm eff}$:

$$\mathcal{Z}_0(\phi) = e^{-\mathcal{H}^{(0)}_{\rm eff}(\phi)} = \text{number of configurations with block average } \phi \tag{1-6}$$

Introducing variables

$$N_\pm(x) \equiv \frac{L^2}{2}[1 \pm \phi(x)] = \text{number of spins in } x \text{ with } s(x) = \pm 1 \tag{1-7}$$

one obtains

$$\mathcal{H}^{(0)}_{\rm eff}(\phi) = -\ln \prod_{x\in\Lambda'} \binom{L^2}{N_\pm(x)} = -\sum_{x\in\Lambda'} \ln \binom{L^2}{\frac{1}{2}L^2(1\pm\phi(x))} \tag{1-8}$$

$\mathcal{H}(s)$ is a sum over contributions associated with links $b = (z, z+\hat{\mu})$.

$$\begin{aligned} -\mathcal{H}(s) &= \sum_{b\in\Lambda} h_b(s) \\ h_b(s) &= s(z)s(z+\hat{\mu}) \quad \text{for} \quad b = (z, z+\hat{\mu}) \end{aligned} \tag{1-9}$$

Since $h_b = \pm 1$

$$\begin{aligned} \langle e^{-\beta\mathcal{H}(s)}\rangle_{\phi,\beta=0} &= \langle \prod_{b\in\Lambda} e^{\beta h_b(s)}\rangle_{\phi,\beta=0} \\ &= (\cosh\beta)^{|\Lambda|} \langle \prod_{b\in\Lambda} [1 + \tanh\beta \cdot h_b(s)]\rangle_{\phi,\beta=0} \end{aligned} \tag{1-10}$$

Here $|\Lambda|$ denotes the number of links b in Λ. We now define "partition functions" $B(X|\phi)$ for all subsets X of links in Λ:

$$B(X|\phi) \equiv \langle \prod_{b\in X} [1 + \tanh\beta \cdot h_b(s)]\rangle_{\phi,\beta=0} \tag{1-11}$$

With this definition we have

$$\mathcal{H}_{\rm eff}(\phi) = \mathcal{H}^{(0)}_{\rm eff}(\phi) - |\Lambda|\ln(\cosh\beta) - \ln B(\Lambda|\phi) \tag{1-12}$$

The Möbius inversion provides a possibility to express $\ln B(\Lambda|\phi)$ as a sum over contributions associated with subsets $\emptyset \neq X \subseteq \Lambda$.

$$\begin{aligned} \ln B(\Lambda|\phi) &= \sum_{\emptyset\neq X\subseteq\Lambda} H(X|\phi) \\ H(X|\phi) &= \sum_{\emptyset\neq Y\subseteq X} (-1)^{|X|-|Y|} \ln B(Y|\phi) \end{aligned} \tag{1-13}$$

The simple proof of this helpful formula can e.g. be found in [15]. We will call the sets of links $X \subseteq \Lambda$ *lattice graphs*, and the $H(X|\phi)$ will be called *Möbius amplitudes*. We will now prove that the Möbius amplitudes of non-connected lattice graphs vanish. A graph is called connected if all blocks which are met by its links are connected. Two blocks are called connected (with respect to the graph X) if there exists at least one link $b \in X$ which meets both blocks. If a lattice graph is not connected then the assumption of the following propositon is valid.

Proposition: If a lattice graph X is disjoint union of two subgraphs, $X = X_1 + X_2$, and if $B(Y_1 + Y_2) = B(Y_1)B(Y_2)$ for all $Y_1 \subseteq X_1$, $Y_2 \subseteq X_2$, then the Möbius amplitude associated with X vanishes, i.e. $H(X) = 0$.

Proof: It follows from the definition of the Möbius amplitudes that

$$(-1)^{|X|}H(X) = \sum_{\emptyset\neq Y\subseteq X} (-1)^{|Y|} \ln B(Y) \tag{1-14}$$

Let us consider the sum over all nonempty subsets $Y \subseteq X$ as decomposed into three groups: (1) all Y which are entirely contained in X_1, (2) all Y which are entirely contained in X_2 and (3) all subsets which have nonempty section with X_1 and X_2. The latter can be regarded as disjoint unions of subsets belonging to group 1 with subsets belonging to group 2. Because of the assumed factorization properties it follows that

$$(-1)^{|X|}H(X) = \sum_{\emptyset \neq Y_1 \subsetneq X_1} (-1)^{|Y_1|} \ln B(Y_1) + \sum_{\emptyset \neq Y_2 \subsetneq X_2} (-1)^{|Y_2|} \ln B(Y_2) + \sum_{\emptyset \neq Y_1 \subsetneq X_1} \sum_{\emptyset \neq Y_2 \subsetneq X_2} (-1)^{|Y_1|+|Y_2|} [\ln B(Y_1) + \ln B(Y_2)] \tag{1-15}$$

We summarize:

$$(-1)^{|X|}H(X) = (-1)^{|X_1|} H(X_1) \left[1 + \sum_{\emptyset \neq Y_2 \subsetneq X_2} (-1)^{|Y_2|} \right] + (1 \to 2) \tag{1-16}$$

But

$$1 + \sum_{\emptyset \neq Y \subsetneq X} (-1)^{|Y|} = \sum_{|Y|=0}^{|X|} \binom{|X|}{|Y|} (-1)^{|Y|} = (1-1)^{|X|} = \delta_{|X|,0} \tag{1-17}$$

Since Möbius amplitudes $H(X)$ are defined for nonempty subsets X only, $|X| = 0$ does not contribute, and the proof is complete.

The quanitities $H(X|\phi)$ are alternating sums of activities $\ln B(Y|\phi)$. These activities can further be decomposed in terms of elementary correlation functions:

$$B(Y|\phi) = \langle \prod_{b \in Y} [1 + \tanh\beta \cdot h_b(s)] \rangle_{\phi,\beta=0} = \sum_{\emptyset \subseteq P \subseteq Y} (\tanh\beta)^{|P|} \langle \prod_{b \in P} h_b(s) \rangle_{\phi,\beta=0} \tag{1-18}$$

The subsets P are the fundamental Mayer graphs. The contribution of the empty set is 1. We now give explicit formulae for the Möbius amplitudes with $|X| \leq 2$:

$$H(\{b\}|\phi) = \ln B(\{b\}|\phi) = \ln(1 + \tanh\beta \cdot \langle h_b \rangle_\cdot) \tag{1-19}$$

$$\begin{aligned} H(\{b_1,b_2\}|\phi) &= \ln B(\{b_1,b_2\}|\phi) - \ln B(\{b_1\}|\phi) - \ln B(\{b_2\}|\phi) \\ &= \ln\left(\frac{1 + \tanh\beta \cdot [\langle h_{b_1} \rangle_\cdot + \langle h_{b_2} \rangle_\cdot] + \tanh^2\beta \cdot \langle h_{b_1} h_{b_2} \rangle_\cdot}{1 + \tanh\beta \cdot [\langle h_{b_1} \rangle_\cdot + \langle h_{b_2} \rangle_\cdot] + \tanh^2\beta \cdot \langle h_{b_1} \rangle_\cdot \langle h_{b_2} \rangle_\cdot} \right) \end{aligned} \tag{1-20}$$

We defined $\langle \mathcal{O} \rangle_\cdot \equiv \langle \mathcal{O} \rangle_{\phi,\beta=0}$. The partition functions $B(Y|\phi)$ are sums of products of correlation functions

$$K_n[\phi(x)] \equiv \langle s(z_1) s(z_2) \dots s(z_n) \rangle_{\phi,\beta=0} \tag{1-21}$$

The lattice sites $z_1, z_2, \dots, z_n$ belong to block x and are mutually distinct. It is easy to see that the K_n do not depend on the positions of the z_i but only on n, on the block spin and on the block size L.

$$\langle \prod_{b \in P} h_b(s) \rangle_{\phi,\beta=0} = \prod_{x : v(P|x) \neq 0} K_{v(P|x)}[\phi(x)] \tag{1-22}$$

The product in Eq. (1-22) runs over all blocks x which are met by the graph P, and

$$v(P|x) \equiv \text{ number of even vertices of } P \text{ in } x \tag{1-23}$$

A vertex is called even (odd) if the number of entering links is even (odd). We will now derive a generating function for the K_n. Because of the Kronecker-δ in the measure $\langle(\cdot)\rangle_{\phi,\beta=0}$

$$e^{\lambda M} = \langle \prod_{i=1}^{l} e^{\lambda s_i} \rangle_{\phi,\beta=0} \tag{1-24}$$

$l \equiv L^2$ denotes the volume of a block and $M \equiv l\phi$ is the block magnetization. Now the "Mayer trick" can be applied:

$$\begin{aligned} e^{\lambda M} &= (\cosh\lambda)^l \langle \prod_{i=1}^{l} [1 + \tanh\lambda \cdot s_i] \rangle_{\phi,\beta=0} \\ &= (\cosh\lambda)^l \sum_{m=0}^{l} \binom{l}{m} (\tanh\lambda)^m \cdot K_m \end{aligned} \tag{1-25}$$

Introducing variables $z \equiv \tanh\lambda$ one obtains a generating function for the K_n:

$$(1+z)^{\frac{1}{2}(l+M)} \cdot (1-z)^{\frac{1}{2}(l-M)} = \sum_{m=0}^{l} \frac{l!\, K_m}{(l-m)!} \frac{z^m}{m!} \tag{1-26}$$

It follows that

$$K_n = \frac{(l-n)!}{l!} \left(\frac{d}{dz}\right)^n [(1+z)^{\frac{1}{2}(l+M)} \cdot (1-z)^{\frac{1}{2}(l-M)}]\Big|_{z=0} \tag{1-27}$$

The differentiation in Eq. (1-27) can comfortably be performed with the help of the computer algebra program REDUCE [47]. The following table shows the K_n for $n \leq 6$:

$$
\begin{aligned}
K_0 &= 1 \\
K_1 &= \phi \\
K_2 &= \frac{l\phi^2 - 1}{l - 1} \\
K_3 &= \frac{l^2\phi^3 - (3l-2)\phi}{(l-1)(l-2)} \\
K_4 &= \frac{l^3\phi^4 - (6l^2 - 8l)\phi^2 + 3l - 6}{(l-1)(l-2)(l-3)} \\
K_5 &= \frac{l^4\phi^5 - (10l^3 - 20l^2)\phi^3 + 15l^2 - 50l + 24}{(l-1)(l-2)(l-3)(l-4)} \\
K_6 &= \frac{l^5\phi^6 - (15l^4 - 40l^3)\phi^4 + (45l^3 - 210l^2 + 184l)\phi^2 - 15l^2 + 90l - 120}{(l-1)(l-2)(l-3)(l-4)(l-5)}
\end{aligned}
\tag{1-28}
$$

An expansion in powers of β can be obtained by a suitable expansion of the Möbius amplitudes. For $|X| \leq 2$

$$
\begin{aligned}
\ln(\cosh\beta) &= \frac{\beta^2}{2} + O(\beta^4) \\
H(\{b\}|\phi) &= \langle h_b \rangle_{\phi,\beta=0} \cdot \beta - \frac{\langle h_b \rangle^2_{\phi,\beta=0}}{2} \cdot \beta^2 + O(\beta^3) \\
H(\{b_1, b_2\}|\phi) &= \langle h_{b_1} h_{b_2} \rangle^T_{\phi,\beta=0} \cdot \beta^2 + O(\beta^3)
\end{aligned}
\tag{1-29}
$$

The remainder of this section is devoted to an explicite high temperature expansion for the effective potential $\mathcal{V}_{\text{eff}}(\phi)$.

$$
\mathcal{V}_{\text{eff}}(\phi) \equiv \mathcal{H}_{\text{eff}}(\phi)|_{\phi=\text{const}}/|\Lambda'| \tag{1-30}
$$

The tables A-1 and A-2 below show all non-equivalent lattice graphs X with $|X| \leq 2$. In addition the multiplicities and the associated Möbius amplitudes are displayed. For the effective potential we choose the parametrization

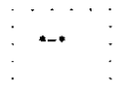
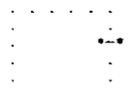
$$
\begin{aligned}
\mathcal{V}_{\text{eff}}(\phi) &= \mathcal{V}^{(0)}_{\text{eff}}(\phi) + \beta \cdot \mathcal{V}^{(1)}_{\text{eff}}(\phi) + \beta^2 \cdot \mathcal{V}^{(2)}_{\text{eff}}(\phi) + O(\beta^3) \\
\mathcal{V}^{(n)}_{\text{eff}}(\phi) &\equiv \sum_{j=0}^{n} \mathcal{V}^{(n)}_{2j} \phi^{2j}
\end{aligned}
\tag{1-31}
$$

For the coefficients one obtains

$$
\mathcal{V}^{(0)}(\phi) = -\ln \binom{L^2}{\frac{1}{2}L^2(1 \pm \phi)}
$$

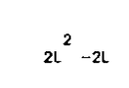
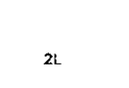
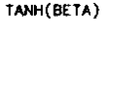
$$
\begin{aligned}
\mathcal{V}^{(1)}_0 &= \frac{2L}{L+1} \\
\mathcal{V}^{(1)}_2 &= \frac{-2L(L^2 + L + 1)}{L+1} \\
\mathcal{V}^{(2)}_0 &= \frac{L^2(-L^5 - L^4 + 6L^3 + 2L^2 - 9L + 1)}{L^5 + L^4 - 4L^3 - 4L^2 + 3L + 3} \\
\mathcal{V}^{(2)}_2 &= \frac{2L^2(L^7 + L^6 - 6L^5 - 4L^4 + 9L^3 + 3L^2 + 10)}{L^7 + L^6 - 6L^5 - 6L^4 + 11L^3 + 11L^2 - 6L - 6} \\
\mathcal{V}^{(2)}_4 &= \frac{L^2(-L^7 - L^6 + 4L^5 + 4L^4 + 3L^3 - 3L^2 - 18L - 18)}{L^7 + L^6 - 6L^5 - 6L^4 + 11L^3 + 11L^2 - 6L - 6}
\end{aligned}
\tag{1-32}
$$

TABLE A-1: Mayer Graphs with |X| = 1

lattice graph	number / block	a
A1 	$2L^2 - 2L$	K2
A2 	$2L$	$K1^2$

V(X) = LOG(1+Ta) , T = TANH(BETA)

TABLE A-2: Mayer Graphs with |X| = 2

lattice graph	number / block	a	b	c
B1 	$2L^4 - 4L^3 - 5L^2 + 13L - 4$	2K2	K4	$K2^2$
B2 	$6L^2 - 12L + 4$	2K2	K2	$K2^2$
B3 	$8L^3 - 8L^2 - 12L + 8$	$K2+K1^2$	K1K3	$K1^2 K2$
B4	$12L - 8$	$K2+K1^2$	$K1^2$	$K1^2 K2$
B5	$6L^2 - 4$	$2K1^2$	$K1^2 K2$	$K1^4$
B6	$L^2 - L$	$2K1^2$	$K2^2$	$K1^4$
B7	4	$2K1^2$	$K1^2$	$K1^4$

$V(X) = LOG(1+aT+bT^2) - LOG(1+aT+cT^2)$, T = TANH(BETA)

A.2. $O(\beta)$ Expansion for the Effective Hamiltonian of the O(N) Model

The first order coefficients of a high temperature expansion for the effective Hamiltonian of the O(N) nonlinear σ-model can be evaluated exactly for all dimensions d and for all N.

$\mathcal{H}^{(1)}_{\rm eff}(\phi)$ is the $O(\beta)$ coefficient of a Mayer expansion for the effective Hamiltonian $\mathcal{H}_{\rm eff}(\phi)$,

$$\mathcal{H}^{(1)}_{\rm eff}(\phi) = \frac{\partial}{\partial\beta}\mathcal{H}_{\rm eff}(\phi)\Big|_{\beta=0} = \langle\mathcal{H}(s)\rangle_{\phi,\beta=0} \tag{2-1}$$

With the decomposition of the fundamental Hamiltonian

$$\begin{aligned}\mathcal{H}(s) &= \sum_{x\in\Lambda'}\mathcal{H}_x(s)\\ \mathcal{H}_x(s) &\equiv -\sum_{z\in x}\sum_{\mu=1}^{d} s(z)\cdot s(z+\hat\mu)\end{aligned} \tag{2-2}$$

it follows that

$$\begin{aligned}\mathcal{H}^{(1)}_{\rm eff}(\phi) &= \sum_{x\in\Lambda'}\langle\mathcal{H}_x(s)\rangle_{\phi,\beta=0}\\ \langle\mathcal{H}_x(s)\rangle_{\phi,\beta=0} &= -\sum_{z\in x}\sum_{\mu=1}^{d}\langle s(z)\cdot s(z+\hat\mu)\rangle_{\phi,\beta=0}\end{aligned} \tag{2-3}$$

In this sum only two distinct contributions occur (cf. graphs A1 and A2 in Table A-1).

$$\langle s(z)\cdot s(z+\hat\mu)\rangle_{\phi,\beta=0} \equiv \begin{cases} K(\phi|x) & \text{if} \quad z\in x,\ z+\hat\mu\in x\\ K_\mu(\phi|x) & \text{if} \quad z\in x,\ z+\hat\mu\in x+\hat\mu'\end{cases} \tag{2-4}$$

$\hat\mu'$ denotes the unit vector in μ-direction on the block lattice Λ'. With these abbreviations

$$\langle\mathcal{H}_x(s)\rangle_{\phi,\beta=0} = -d(L^d - L^{d-1})\,K(\phi|x) - L^{d-1}\sum_{\mu=1}^{d}K_\mu(\phi|x) \tag{2-5}$$

The correlation functions $K(\phi|x)$ and $K_\mu(\phi|x)$ can be evaluated exactly. Let us first consider $K_\mu(\phi|x)$: Since the two spins belong to different blocks and the expectation value $\langle(\cdot)\rangle_{\phi,\beta=0}$ factorizes

$$\begin{aligned}K_\mu(x|\phi) &= \langle s(z)\cdot s(z+\hat\mu)\rangle_{\phi,\beta=0}\\ &= \langle s(z)\rangle_{\phi,\beta=0}\cdot\langle s(z+\hat\mu)\rangle_{\phi,\beta=0}\\ &= \lambda^{-2}\phi(x)\cdot\phi(x+\hat\mu')\\ &= L^{2-d}\phi(x)\cdot\phi(x+\hat\mu')\end{aligned} \tag{2-6}$$

$K(x|\phi)$ can be derived using a simple trick [28]:

$$\begin{aligned}\lambda^{-2}\phi(x)^2 &= \langle\Big|\sum_{z\in x}s(z)\Big|^2\rangle_{\phi,\beta=0}\\ &= L^{-2d}\sum_{v\in x}\sum_{w\in x}\langle s(v)\cdot s(w)\rangle_{\phi,\beta=0}\\ &= L^{-2d}[L^d - L^d(L^d-1)K(x|\phi)]\end{aligned} \tag{2-7}$$

If this is solved for $K(x|\phi)$ one finds

$$K(x|\phi) = \frac{L^2\phi(x)^2 - 1}{L^d - 1} \tag{2-8}$$

Thus

$$H_1(\phi) = -d(L^d - L^{d-1})\sum_{x\in\Lambda'}\frac{L^2\phi(x)^2-1}{L^d-1} - L\sum_{x\in\Lambda'}\sum_{\mu=1}^{d}\phi(x)\cdot\phi(x+\hat\mu') \tag{2-9}$$

We now consider the special case that the block spin is constant. Then the $O(\beta)$ coefficient of the effective potential $\mathcal{V}^{(1)}_{\rm eff}(\phi)$ is given by

$$\mathcal{V}^{(1)}_{\rm eff}(\phi) = -\frac{dL^d}{L^d-1}\left[(L^2 - L^{1-d})\phi^2 - (1-L^{-1})\right] \tag{2-10}$$

Finally we focus our attention to two dimensions:

$$\mathcal{V}^{(1)}_{\rm eff}(\phi)\big|_{d=2} = -\frac{2L}{L+1}\left[(L^2+L+1)\phi^2 - 1\right] \tag{2-11}$$

A.3. Computation of Mayer Coefficients by Monte Carlo Simulations with $\beta = 0$

Using the Monte Carlo method developed in Chapter II one can also compute coefficients of a Mayer expansion for the effective Hamiltonian. To do this one has to determine truncated moments of the fundamental Hamiltonian at $\beta = 0$ with fixed block spins ϕ. We apply the procedure for the effective potential of the Ising model and the O(3) model in two dimensions. The results are compared with results from analytical calculations (Appendix A.1. for the Ising model and [28] for the O(3) model).

We start from the identity

$$\frac{e^{-\mathcal{H}_{\text{eff}}(\phi)}}{e^{-\mathcal{H}^{(0)}_{\text{eff}}(\phi)}} = \langle e^{-\beta\mathcal{H}(s)}\rangle_{\phi,\beta=0} \tag{3-1}$$

The abbreviations used in this section were defined in Chapter II and in Appendix A.1.

$$\begin{aligned}\mathcal{H}_{\text{eff}}(\phi) &= \mathcal{H}^{(0)}_{\text{eff}}(\phi) - \sum_{n\geq 1}\frac{(-\beta)^n}{n!}\langle\mathcal{H}(s)^n\rangle^T_{\phi,\beta=0} \\ &\equiv \sum_{n\geq 0}\beta^n\,\mathcal{H}^{(n)}_{\text{eff}}(\phi)\end{aligned} \tag{3-2}$$

For $n \geq 1$

$$\mathcal{H}^{(n)}_{\text{eff}}(\phi) = \frac{(-1)^{n+1}}{n!}\cdot\langle\mathcal{H}(s)^n\rangle^T_{\phi,\beta=0} \tag{3-3}$$

Therefore in principle one can compute the $\mathcal{H}^{(n)}_{\text{eff}}(\phi)$ using the Monte Carlo method worked out in Chapter II. However this will work only for small n. Since the energy $\mathcal{H}(s)$ is an extensive quantity the moments of $\mathcal{H}$ will show strong fluctuations when the lattice volume is increased. The Monte Carlo estimates therefore will suffer from large statistical errors. This situation can be considerably improved by taking advantage of the fact that the measure $\langle(\cdot)\rangle_{\phi,\beta=0}$ factorizes over the blocks $x \in \Lambda'$. Using the decomposition Eq. (2-2) of $\mathcal{H}(s)$ it follows from the properties of truncated expectation values that in the sum

$$\langle\mathcal{H}(s)^n\rangle_{\phi,\beta=0} = \sum_{x_1\in\Lambda'}\cdots\sum_{x_n\in\Lambda'}\langle\mathcal{H}_{x_1}(s)\ldots\mathcal{H}_{x_n}(s)\rangle^T_{\phi,\beta=0} \tag{3-4}$$

only terms contribute where the sites $\{x_1,\ldots,x_n\}$ are connected in the block lattice, e.g.

$$\begin{aligned}\mathcal{H}^{(2)}_{\text{eff}}(\phi) &= -\frac{1}{2}\sum_x\sum_y\langle\mathcal{H}_x(s)\mathcal{H}_y(s)\rangle^T_{\phi,\beta=0} \\ &= -\frac{1}{2}\Big[\sum_x\langle\mathcal{H}_x(s)^2\rangle^T_{\phi,\beta=0} + 2\sum_x\sum_{\mu=1}^{d}\langle\mathcal{H}_x(s)\mathcal{H}_{x+\hat{\mu}}(s)\rangle^T_{\phi,\beta=0}\Big]\end{aligned} \tag{3-5}$$

For $n = 2$ and for $n = 3$ one can take advantage of the fact that

$$\begin{aligned}\langle\mathcal{H}_x\mathcal{H}_y\rangle^T &= \langle(\mathcal{H}_x - \langle\mathcal{H}_x\rangle)(\mathcal{H}_y - \langle\mathcal{H}_y\rangle)\rangle \\ \langle\mathcal{H}_x\mathcal{H}_y\mathcal{H}_z\rangle^T &= \langle(\mathcal{H}_x - \langle\mathcal{H}_x\rangle)(\mathcal{H}_y - \langle\mathcal{H}_y\rangle)(\mathcal{H}_z - \langle\mathcal{H}_z\rangle)\rangle\end{aligned} \tag{3-6}$$

(Such a formula is *not* valid for $n > 3$. However, there exists a generalization with complex coefficients, see Appendix B.2.) Since the expectation values $\langle\mathcal{H}_x\rangle_{\phi,\beta=0}$ are exactly known (see Appendix A.2.) the reduction to the truncated part can be done at "Monte Carlo time". Furthermore, if Mayer coefficients for the effective potential are computed the expectation values $\langle(\cdot)\rangle_{\phi,\beta=0}$ are translationally invariant.

For Monte Carlo simulations to compute Mayer coefficients of $O(\beta^n)$ the side length of the block lattice must exceed $n+1$, otherwise certain Mayer graphs might overlap themselves.

The following tables show Monte Carlo results for the coefficients $\mathcal{V}^{(2)}_{\text{eff}}(\phi)$ of the Ising model (Table A-3) and of the O(3) model (Table A-4) on a 2-dimensional lattice.

Table A-3: $\mathcal{V}^{(2)}_{\text{eff}}(\phi)$ for the d=2 Ising Model

ϕ	Monte Carlo	analytically	consistency
	L=4		
0/8	-14.723 (69)	-14.753	yes
1/8	-14.180 (66)	-14.246	yes
2/8	-12.754 (42)	-12.779	yes
3/8	-10.478 (44)	-10.510	yes
4/8	-7.689 (46)	-7.700	yes
5/8	-4.738 (21)	-4.719	yes
6/8	-2.054 (19)	-2.039	yes
7/8	-0.235 (05)	-0.238	yes

The Monte Carlo results are based on simulations of the 2-dimensional Ising model with fixed constant block spin at $\beta = 0$. The block lattice was 3×3. 10 groups of 5000 sweeps were performed (CPU 6 minutes on [49]). The numbers in the column "analytically" are results of an analytical Mayer expansion for the effective potential (Section A.1. of this appendix). Within the statistical errors the numerical and the analytical data are consistent.

Table A-4: $\mathcal{V}_{\rm eff}^{(2)}(\phi)$ for the d=2 O(3) Model

ϕ	Monte Carlo	analytically	consistency
L=2			
0.0	-1.4505 (52)	-	-
0.1	-1.2838 (27)	-	-
0.2	-1.1125 (37)	-	-
0.3	-0.9353 (37)	-	-
0.4	-0.7672 (42)	-	-
0.5	-0.6157 (25)	-	-
0.6	-0.4803 (15)	-	-
0.7	-0.3334 (07)	-	-
0.8	-0.1779 (06)	-	-
0.9	-0.0528 (02)	-	-
L=4			
0.0	-4.856 (52)	-4.907	yes
0.1	-4.777 (43)	-4.802	yes
0.2	-4.502 (34)	-4.496	yes
0.3	-3.993 (32)	-4.022	yes
0.4	-3.448 (24)	-3.445	yes
0.5	-2.751 (19)	-2.853	yes
0.6	-2.079 (11)	-2.384	no
0.7	-1.392 (09)	-	-
0.8	-0.761 (06)	-	-
0.9	-0.231 (01)	-	-
L=6			
0.0	-11.63 (13)	-11.51	yes
0.1	-11.27 (14)	-11.27	yes
0.2	-10.60 (09)	-10.58	yes
0.3	-9.60 (09)	-9.51	yes
0.4	-8.15 (08)	-8.19	yes
0.5	-6.64 (08)	-6.80	no
0.6	-4.86 (05)	-5.62	no
0.7	-3.32 (05)	-	-
0.8	-1.82 (02)	-	-
0.9	-0.55 (01)	-	-

Table A-4: $\mathcal{V}_{\rm eff}^{(2)}(\phi)$ for the O(3) Model, Continuation

ϕ	Monte Carlo	analytically	consistency
L=8			
0.0	-21.05 (29)	-20.81	yes
0.1	-20.17 (31)	-20.38	yes
0.2	-19.73 (21)	-19.16	yes
0.3	-17.18 (23)	-17.25	yes
0.4	-14.61 (17)	-14.86	yes
0.5	-12.12 (15)	-12.33	no
0.6	-9.27 (14)	-10.14	no
0.7	-6.00 (07)	-	-
0.8	-3.27 (05)	-	-
0.9	-1.00 (01)	-	-
L=10			
0.0	-32.23 (58)	-32.78	yes
0.1	-32.22 (29)	-32.12	yes
0.2	-30.48 (56)	-30.20	yes
0.3	-27.03 (55)	-27.20	yes
0.4	-22.99 (23)	-23.45	no
0.5	-18.65 (20)	-19.45	no
0.6	-13.87 (26)	-15.96	no
0.7	-9.39 (11)	-	-
0.8	-5.16 (08)	-	-
0.9	-1.59 (02)	-	-

The Monte Carlo results are based on simulations of the 2-dimensional O(3) model with fixed constant block spin ϕ at $\beta = 0$. $|\Lambda'|$ was a 4×4 lattice. 10 groups of $10^4/L^2$ sweeps were performed (CPU 63 minutes on [49]). The numbers in the column "analytically" are based on the analytical Mayer expansion for the effective potential in [28]. The missing consistency for $\phi > 0.5$ is due to an approximation used in the analytical calculations which becomes worse for large block spin. In [28] no results are given for $\phi > 0.6$.

Appendix B: Supplement to Chapter III

B.1. *Composition of Linear Gaussian Block Spin Transformations*

B.2. *Truncated Correlation Functions as Simple Correlation Functions in a Multiplied System*

B.3. *Tables of Quadratic Taylor Coefficients for the Effective Hamiltonian of the 2-Dimensional Ising Model*

B.1. Composition of Linear Gaussian Block Spin Transformations

Composition rules for linear Gaussian block spin transformations are derived. Compositions of such transformations are again Gaussian block spin transformations (with changed parameters).

A linear Gaussian block spin transformation for a real N-vector field ϕ on a cubic d-dimensional lattice Λ is determined by the (normalized) block spin probability distribution

$$\begin{aligned} P^{\kappa,b}(\phi'|\phi) &\equiv \prod_{x'\in\Lambda'} P^{\kappa,b}_{x'}(\phi'|\phi) \\ P^{\kappa,b}_{x'}(\phi'|\phi) &\equiv \frac{e^{-\frac{1}{2}\kappa[\phi'(x')-b\sum_{x\in x'}\phi(x)]^2}}{(2\pi/\kappa)^{N/2}} \end{aligned} \tag{1-1}$$

We consider dimensionless fields ϕ. Therefore also the parameter κ is dimensionless. All the following considerations remain valid in the limit $\kappa \to \infty$ (δ block spin).

The composition of two successive block spin transformations with scale factors L_1 and L_2 is a convolution of two Gaussian distributions which is again a Gaussian distribution. Therefore it is legitimate to write

$$P^{\kappa_{12},b_{12}}_{x''}(\phi''|\phi) = \int \prod_{x'\in x''} d^N\phi'(x') \cdot P^{\kappa_2,b_2}_{x''}(\phi''|\phi') \cdot \prod_{x'\in x''} P^{\kappa_1,b_1}_{x'}(\phi'|\phi) \tag{1-2}$$

In this appendix it will be shown that the parameters κ_{12} and b_{12} for the composed transformation are given by

$$\begin{aligned} \frac{1}{\kappa_{12}} &= \frac{1}{\kappa_2} + \frac{b_2^2 L_2^d}{\kappa_1} \\ b_{12} &= b_1 \cdot b_2 \end{aligned} \tag{1-3}$$

We use the formula

$$\frac{e^{-\frac{1}{2}\alpha x^2}}{(2\pi/\alpha)^{N/2}} = \int \frac{d^Nk}{(2\pi)^N} e^{-\frac{1}{2}k^2/\alpha} e^{ikx} \tag{1-4}$$

to represent $P^{\kappa_2,b_2}_{x''}(\phi''|\phi')$. The r.h.s. of Eq. (1-2) is

$$\begin{aligned} \text{r.h.s.} = &\int \frac{d^Nk}{(2\pi)^N} e^{-\frac{1}{2}k^2/\kappa_2} \cdot e^{ik\phi''(x'')} \\ &\cdot \int \prod_{x'\in x''} d^N\phi'(x') \cdot e^{-ikb_2\sum_{x'\in x''}\phi'(x')} \prod_{x'\in x''} \frac{e^{-\frac{1}{2}\kappa_1[\phi'(x')-b_1\sum_{x\in x'}\phi(x)]^2}}{(2\pi/\kappa_1)^{N/2}} \end{aligned} \tag{1-5}$$

After a translation $\phi'(x') \to \phi'(x') + b_1\sum_{x\in x'}\phi(x)$ the ϕ'-integrations factorize:

$$\text{r.h.s.} = \int \frac{d^Nk}{(2\pi)^N} e^{-\frac{1}{2}k^2/\kappa_2} e^{ik[\phi''(x'')-b_1b_2\sum_{x\in x''}\phi(x)]} \Big[\int d^N\phi' e^{-ikb_2\phi'} \frac{e^{-\frac{1}{2}\kappa_1\phi'^2}}{(2\pi/\kappa_1)^{N/2}}\Big]^{L_2^d} \tag{1-6}$$

Using the formula

$$\int d^Nx \frac{e^{-\frac{1}{2}\alpha x^2+i\kappa x}}{(2\pi/\alpha)^{N/2}} = e^{-\frac{1}{2}\kappa^2/\alpha} \tag{1-7}$$

we find

$$\begin{aligned} \text{r.S.} &= \int \frac{d^Nk}{(2\pi)^N} e^{-\frac{1}{2}k^2[\frac{1}{\kappa_2}+\frac{b_2^2L_2^d}{\kappa_1}]} e^{ik[\phi''(x'')-b_1b_2\sum_{x\in x''}\phi(x)]} \\ &= \frac{e^{-\frac{1}{2}\kappa_{12}[\phi''(x'')-b_{12}\sum_{x\in x''}\phi(x)]^2}}{(2\pi/\kappa_{12})^{N/2}} \end{aligned} \tag{1-8}$$

From this Eq. (1-3) is obvious.

Let us now determine the parameters κ_k, b_k for a renormalization group transformation which is equivalent to k successive transformations with always the same scale factor L and always the same parameters κ, b. One considers the transformation as composed of a step with block size L^{k-1} and a subsequent single transformation with scale factor L. Equation (1-3) says:

$$\frac{1}{\kappa_k} = \frac{1}{\kappa} + \frac{b^2L^d}{\kappa_{k-1}} \tag{1-9}$$

This relation can easily be iterated:

$$\frac{\kappa}{\kappa_k} = 1 + b^2 L^d \frac{\kappa}{\kappa_{k-1}} = 1 + b^2 L^2 [1 + b^2 L^2 [\dots$$
$$= \sum_{n=0}^{k-1} (b^2 L^d)^n \tag{1-10}$$
$$= \frac{1 - (b^2 L^d)^k}{1 - b^2 L^d}$$

This result can also be derived if one starts from a more general consideration: The transformations P^{κ_1, b_1} and P^{κ_2, b_2} commute if and only if

$$\frac{\kappa_1}{\kappa_2} = \frac{1 - b_2^2 L_2^d}{1 - b_1^2 L_1^d} \tag{1-11}$$

One can use this identity to eliminate the parameter κ_2 in the equation

$$\kappa_{12} = \frac{\kappa_1 \kappa_2}{\kappa_1 + b_2^2 L_2^d \kappa_2} \tag{1-12}$$

with the result

$$\kappa_{12} = \kappa_1 \cdot \frac{1 - b_1^2 L_1^d}{1 - (b_1 b_2)^2 (L_1 L_2)^d} \tag{1-13}$$

Inserting $L_1 = L$ and $L_2 = L^{k-1}$ Eq. (1-10) is recovered.

B.2. Truncated Correlation Functions as Simple Correlation Functions in a Multiplied System

It is shown that truncated n-point correlation functions of a statistical mechanical system can be expressed as simple correlation functions of modified observables in a suitably chosen auxiliary system. This auxiliary system consists of n copies of the original system which do not interact. The identy derived is a generalization of the well known "doubling trick" for truncated 2-point functions.

Let $O_1, O_2, \dots, O_n$ be a set of observables in some statistical mechanical system. The truncated correlation function for the product of the observables is defined by

$$\langle \prod_{i=1}^{n} O_i \rangle^T \equiv \left(\prod_{i=1}^{n} \frac{\partial}{\partial h_i} \right) \ln \langle e^{\sum_{i=1}^{n} h_i O_i} \rangle \Big|_{h=0} \tag{2-1}$$

E.g., for $n = 2$:

$$\langle O_1 O_2 \rangle^T = \langle O_1 O_2 \rangle - \langle O_1 \rangle \langle O_2 \rangle \tag{2-2}$$

Let us now consider the union of n identical copies of the system. Quantities which refer to the i-th copy will be labeled by an index (i). Since the systems are identical

$$\langle O_i^{(1)} \rangle_{(1)} = \langle O_i^{(2)} \rangle_{(2)} = \cdots = \langle O_i^{(n)} \rangle_{(n)} = \langle O_i \rangle \tag{2-3}$$

The systems do not interact with each other. Therefore expectation values of observables which refer to different systems factorize. E.g.,

$$\langle \langle O_i^{(1)} O_j^{(2)} \rangle_{(1)} \rangle_{(2)} = \langle O_i^{(1)} \rangle_{(1)} \cdot \langle O_j^{(2)} \rangle_{(2)} = \langle O_i \rangle \langle O_j \rangle \tag{2-4}$$

The expectation value in the n-fold system will be denoted by

$$[\![(\cdot)]\!] \equiv \langle \dots \langle \langle (\cdot) \rangle_{(1)} \rangle_{(2)} \dots \rangle_{(n)} \tag{2-5}$$

The proposition stated below is a generalization of the well known "doubling trick". As a preparation this trick will be briefly presented. For $n = 2$ we define

$$\hat{O}_1 \equiv O_1^{(1)} - O_1^{(2)}$$
$$\hat{O}_2 \equiv O_2^{(1)} - O_2^{(2)} \tag{2-6}$$

Then

$$[\![\hat{O}_1 \hat{O}_2]\!] = [\![O_1^{(1)} O_2^{(1)}]\!] + [\![O_1^{(2)} O_2^{(2)}]\!] - [\![O_1^{(1)} O_2^{(2)}]\!] - [\![O_1^{(2)} O_2^{(1)}]\!]$$
$$= \langle O_1^{(1)} O_2^{(1)} \rangle_{(1)} + \langle O_1^{(2)} O_2^{(2)} \rangle_{(2)} - \langle O_1^{(1)} \rangle_{(1)} \langle O_2^{(2)} \rangle_{(2)} - \langle O_1^{(2)} \rangle_{(2)} \langle O_2^{(1)} \rangle_{(1)} \tag{2-7}$$
$$= 2 \langle O_1 O_2 \rangle^T$$

We now state the following

Proposition: For each of the observables O_k, $k = 1, .., n$ an observable $\hat{O}_k$ is defined which refers to the n-fold system:

$$\hat{O}_k \equiv \sum_{j=1}^{n} \xi^{j-1} O_k^{(j)}$$
$$\xi \equiv e^{2\pi i / n} \tag{2-8}$$

Then

$$\langle \prod_{i=1}^{n} O_i \rangle^T = \frac{1}{n} [\![\prod_{i=1}^{n} \hat{O}_i]\!] \tag{2-9}$$

Proof: Because of the identity of the systems

$$\begin{aligned}\langle\prod_{i=1}^{n} O_i\rangle^T &= \frac{1}{n}\sum_{j=1}^{n}\langle\prod_{i=1}^{n} O_i^{(j)}\rangle_{(j)}^T \\ &= \frac{1}{n}\sum_{j=1}^{n}\left\{\left(\prod_{i=1}^{n}\frac{\partial}{\partial h_i}\right)\ln\langle e^{\sum_{i=1}^{n} h_i O_i^{(j)}}\rangle_{(j)}\right\}_{h=0} \\ &= \frac{1}{n}\left(\prod_{i=1}^{n}\frac{\partial}{\partial h_i}\right)\left\{\sum_{j=1}^{n}\ln\langle e^{\sum_{i=1}^{n} h_i O_i^{(j)}}\rangle_{(j)}\right\}\Big|_{h=0}\end{aligned} \tag{2-10}$$

Since $\xi^n = 1$, the expectation value on the left hand side of Eq. (2-10) is invariant with respect to the transformations $O_i \to \xi^{j-1} O_i$, $j = 1, ..., n$. Therefore it follows from the last line in Eq. (2-10) that

$$\langle\prod_{i=1}^{n} O_i\rangle^T = \frac{1}{n}\left(\prod_{i=1}^{n}\frac{\partial}{\partial h_i}\right)\left\{\sum_{j=1}^{n}\ln\langle e^{\sum_{i=1}^{n} h_i \xi^{j-1} O_i^{(j)}}\rangle_{(j)}\right\}\Big|_{h=0} \tag{2-11}$$

Since the systems (j) are statistically independent

$$\begin{aligned}\sum_{j=1}^{n}\ln\langle e^{\sum_{i=1}^{n} h_i \xi^{j-1} O_i^{(j)}}\rangle_{(j)} &= \ln\prod_{j=1}^{n}\langle e^{\sum_{i=1}^{n} h_i \xi^{j-1} O_i^{(j)}}\rangle_{(j)} \\ &= \ln[\![\prod_{j=1}^{n} e^{\sum_{i=1}^{n} h_i \xi^{j-1} O_i^{(j)}}]\!] \\ &= \ln[\![e^{\sum_{i=1}^{n} h_i \hat{O}_i}]\!]\end{aligned} \tag{2-12}$$

We have thus shown that

$$\langle\prod_{i=1}^{n} O_i\rangle^T = \frac{1}{n}[\![\prod_{i=1}^{n}\hat{O}_i]\!]^T \tag{2-13}$$

We now recognize that

$$[\![\prod_{i=1}^{n}\hat{O}_i]\!]^T = [\![\prod_{i=1}^{n}\hat{O}_i]\!] + R \tag{2-14}$$

R is a weighted sum of products. These products consist of factors which are of the form (eventually after renumbering the observables)

$$r = [\![\prod_{i=1}^{k}\hat{O}_i]\!], \qquad k < n \tag{2-15}$$

It is easy to see that all the r's vanish. Namely,

$$r = \xi^{n-k}[\![\prod_{i=1}^{k}(\xi\hat{O}_i)]\!] \tag{2-16}$$

A simultaneous multiplication of the $\hat{O}_i$ with ξ is equivalent to a cyclic permutation of the system numbers (i). Since this leaves expectation values invariant it follows that $r = \xi^{n-k} r$. We assumed $n \neq k$. Therefore r must vanish. This completes the proof of the proposition.

B.3. Tables of Quadratic Taylor Coefficients for the Effective Hamiltonian of the 2-Dimensional Ising Model

Monte Carlo results for quadratic Taylor coefficients of the effective Hamiltonian for the 2-dimensional Ising model at the critical point are presented.

Tabelle B-3-a: Taylor Coefficients for $\kappa = 6$

Tabelle B-3-b: Taylor Coefficients for $\kappa = 12$

Tabelle B-3-c: Taylor Coefficients for $\kappa = 18$

Identifier	Coefficient	$\|x - y\|$
k_1	$h(x;\phi)$	0
k_2	$h(x,x;\phi)$	0
k_3	$h(x,y;\phi)$	1
k_4	$h(x,y;\phi)$	$\sqrt{2}$
k_5	$h(x,y;\phi)$	2
k_6	$h(x,y;\phi)$	$\sqrt{5}$
k_7	$h(x,y;\phi)$	$\sqrt{8}$
k_8	$h(x,y;\phi)$	3

The statistical errors quoted in the tables were obtained by dividing the data sample into 10 groups.

TABLE B-3-a: Taylor Coefficients, KAPPA = 6

	L = 2	L = 4	L = 8	L = 16
	PHI = 0.0			
k1	0.0001 +/- 0.0011	0.0049 +/- 0.0048	0.0018 +/- 0.0174	-0.0242 +/- 0.0532
k2	-0.1146 +/- 0.0029	-0.5611 +/- 0.0033	-0.4363 +/- 0.0193	-0.3281 +/- 0.0405
k3	-0.8614 +/- 0.0018	-1.0072 +/- 0.0020	-1.0230 +/- 0.0120	-0.9606 +/- 0.0371
k4	-0.1131 +/- 0.0010	-0.2240 +/- 0.0040	-0.2626 +/- 0.0071	-0.2062 +/- 0.0253
k5	0.1178 +/- 0.0009	0.1156 +/- 0.0028	0.1049 +/- 0.0140	0.1096 +/- 0.0317
k6	0.0899 +/- 0.0006	0.0675 +/- 0.0042	0.0597 +/- 0.0074	0.0750 +/- 0.0141
k7	0.0263 +/- 0.0012	0.0174 +/- 0.0045	0.0171 +/- 0.0127	0.0083 +/- 0.0366
k8	-0.0430 +/- 0.0013	-0.0186 +/- 0.0043	-0.0171 +/- 0.0126	-0.0384 +/- 0.0345
	PHI = 0.2			
k1	-0.6849 +/- 0.0013	-0.8595 +/- 0.0046	-0.8201 +/- 0.0174	-0.8781 +/- 0.0372
k2	-0.3593 +/- 0.0020	0.0853 +/- 0.0058	0.2160 +/- 0.0178	0.4266 +/- 0.0433
k3	-0.9652 +/- 0.0017	-0.8770 +/- 0.0033	-0.8570 +/- 0.0117	-0.7981 +/- 0.0211
k4	-0.1716 +/- 0.0014	-0.2094 +/- 0.0040	-0.2155 +/- 0.0089	-0.2254 +/- 0.0161
k5	0.1147 +/- 0.0015	0.0776 +/- 0.0044	0.0738 +/- 0.0056	0.1062 +/- 0.0252
k6	0.0828 +/- 0.0009	0.0439 +/- 0.0029	0.0525 +/- 0.0067	0.0584 +/- 0.0203
k7	0.0235 +/- 0.0012	0.0090 +/- 0.0024	0.0286 +/- 0.0074	0.0179 +/- 0.0298
k8	-0.0302 +/- 0.0014	-0.0080 +/- 0.0036	0.0010 +/- 0.0059	0.0317 +/- 0.0227
	PHI = 0.4			
k1	-1.4929 +/- 0.0012	-1.3243 +/- 0.0048	-1.2618 +/- 0.0067	-1.2424 +/- 0.0099
k2	0.4378 +/- 0.0033	1.5087 +/- 0.0066	1.6170 +/- 0.0143	1.6180 +/- 0.0315
k3	-0.8671 +/- 0.0014	-0.5477 +/- 0.0020	-0.5006 +/- 0.0056	-0.5089 +/- 0.0178
k4	-0.2066 +/- 0.0008	-0.1344 +/- 0.0017	-0.1205 +/- 0.0047	-0.1289 +/- 0.0194
k5	0.0578 +/- 0.0011	0.0326 +/- 0.0019	0.0414 +/- 0.0026	0.0467 +/- 0.0148
k6	0.0348 +/- 0.0006	0.0155 +/- 0.0014	0.0231 +/- 0.0020	0.0186 +/- 0.0137
k7	0.0086 +/- 0.0009	0.0058 +/- 0.0028	0.0094 +/- 0.0037	0.0214 +/- 0.0116
k8	-0.0067 +/- 0.0008	-0.0014 +/- 0.0018	-0.0007 +/- 0.0061	0.0200 +/- 0.0128
	PHI = 0.6			
k1	-1.7566 +/- 0.0010	-1.2579 +/- 0.0019	-1.1397 +/- 0.0058	-1.1134 +/- 0.0147
k2	2.7625 +/- 0.0023	2.7405 +/- 0.0037	2.6461 +/- 0.0119	2.6275 +/- 0.0222
k3	-0.3854 +/- 0.0008	-0.2685 +/- 0.0014	-0.2593 +/- 0.0047	-0.2537 +/- 0.0107
k4	-0.0859 +/- 0.0010	-0.0584 +/- 0.0011	-0.0552 +/- 0.0030	-0.0548 +/- 0.0060
k5	0.0075 +/- 0.0006	0.0094 +/- 0.0008	0.0082 +/- 0.0023	0.0175 +/- 0.0039
k6	0.0033 +/- 0.0006	0.0029 +/- 0.0007	0.0045 +/- 0.0014	0.0065 +/- 0.0046
k7	0.0011 +/- 0.0006	-0.0003 +/- 0.0007	0.0026 +/- 0.0018	0.0020 +/- 0.0058
k8	-0.0012 +/- 0.0006	0.0009 +/- 0.0006	-0.0050 +/- 0.0025	0.0090 +/- 0.0060
	PHI = 0.8			
k1	-1.2267 +/- 0.0006	-0.8047 +/- 0.0011	-0.7255 +/- 0.0040	-0.6577 +/- 0.0312
k2	4.4343 +/- 0.0015	3.4558 +/- 0.0026	3.2759 +/- 0.0077	3.1716 +/- 0.0407
k3	-0.1099 +/- 0.0004	-0.1290 +/- 0.0008	-0.1270 +/- 0.0021	-0.1382 +/- 0.0108
k4	-0.0173 +/- 0.0002	-0.0242 +/- 0.0005	-0.0236 +/- 0.0010	-0.0256 +/- 0.0071
k5	-0.0001 +/- 0.0004	0.0016 +/- 0.0003	0.0008 +/- 0.0013	0.0091 +/- 0.0031
k6	-0.0008 +/- 0.0002	0.0006 +/- 0.0003	0.0016 +/- 0.0013	0.0034 +/- 0.0021
k7	-0.0005 +/- 0.0002	0.0007 +/- 0.0004	0.0003 +/- 0.0017	0.0045 +/- 0.0031
k8	-0.0005 +/- 0.0003	-0.0013 +/- 0.0003	0.0015 +/- 0.0012	0.0013 +/- 0.0017
	PHI = 1.0			
k1	-0.3028 +/- 0.0003	-0.1558 +/- 0.0010	-0.1214 +/- 0.0021	-0.0815 +/- 0.0160
k2	5.2399 +/- 0.0008	3.8532 +/- 0.0017	3.5963 +/- 0.0036	3.4919 +/- 0.0186
k3	-0.0293 +/- 0.0002	-0.0639 +/- 0.0004	-0.0730 +/- 0.0012	-0.0774 +/- 0.0033
k4	-0.0032 +/- 0.0001	-0.0102 +/- 0.0002	-0.0131 +/- 0.0007	-0.0079 +/- 0.0018
k5	-0.0009 +/- 0.0001	0.0003 +/- 0.0003	0.0008 +/- 0.0008	0.0032 +/- 0.0026
k6	-0.0008 +/- 0.0001	-0.0002 +/- 0.0002	-0.0006 +/- 0.0007	0.0011 +/- 0.0015
k7	-0.0008 +/- 0.0002	0.0000 +/- 0.0002	-0.0004 +/- 0.0008	0.0048 +/- 0.0017
k8	-0.0007 +/- 0.0002	-0.0007 +/- 0.0003	-0.0006 +/- 0.0008	0.0018 +/- 0.0037

TABLE B-3-b: Taylor Coefficients, KAPPA = 12

	L = 2	L = 4	L = 8	L = 16
	PHI = 0.0			
k1	-0.0002 +/- 0.0009	0.0002 +/- 0.0031	0.0074 +/- 0.0123	-0.0436 +/- 0.0270
k2	2.0781 +/- 0.0074	-1.0174 +/- 0.0067	-1.0355 +/- 0.0358	-0.9698 +/- 0.0824
k3	-0.6346 +/- 0.0022	-0.9458 +/- 0.0037	-0.9870 +/- 0.0129	-1.0419 +/- 0.0210
k4	0.0297 +/- 0.0019	-0.0145 +/- 0.0027	-0.0359 +/- 0.0139	-0.0468 +/- 0.0344
k5	0.1139 +/- 0.0015	0.2154 +/- 0.0046	0.2351 +/- 0.0141	0.2068 +/- 0.0208
k6	0.0740 +/- 0.0018	0.0741 +/- 0.0021	0.0823 +/- 0.0109	0.0414 +/- 0.0321
k7	0.0046 +/- 0.0016	-0.0127 +/- 0.0047	0.0109 +/- 0.0095	-0.1427 +/- 0.0217
k8	-0.0628 +/- 0.0010	-0.0646 +/- 0.0047	-0.0699 +/- 0.0110	-0.0843 +/- 0.0536
	PHI = 0.2			
k1	-0.2925 +/- 0.0013	-0.7732 +/- 0.0035	-0.7962 +/- 0.0111	-0.8130 +/- 0.0206
k2	-0.9320 +/- 0.0066	-0.8129 +/- 0.0069	-0.7231 +/- 0.0249	-0.5637 +/- 0.0738
k3	-1.0726 +/- 0.0028	-0.9881 +/- 0.0052	-1.0282 +/- 0.0142	-1.0310 +/- 0.0373
k4	-0.0337 +/- 0.0024	-0.0411 +/- 0.0047	-0.0702 +/- 0.0124	-0.1144 +/- 0.0264
k5	0.1948 +/- 0.0024	0.2234 +/- 0.0062	0.2167 +/- 0.0122	0.2521 +/- 0.0317
k6	0.1123 +/- 0.0021	0.0783 +/- 0.0034	0.0855 +/- 0.0093	0.0895 +/- 0.0297
k7	0.0078 +/- 0.0023	-0.0094 +/- 0.0047	0.0120 +/- 0.0169	0.0077 +/- 0.0475
k8	-0.0831 +/- 0.0034	-0.0551 +/- 0.0049	-0.0345 +/- 0.0175	-0.0142 +/- 0.0284
	PHI = 0.4			
k1	-1.2428 +/- 0.0011	-1.5025 +/- 0.0036	-1.4986 +/- 0.0099	-1.4823 +/- 0.0229
k2	-0.4365 +/- 0.0061	0.3248 +/- 0.0120	0.7159 +/- 0.0170	0.7465 +/- 0.0678
k3	-1.0543 +/- 0.0024	-0.9880 +/- 0.0043	-0.9234 +/- 0.0099	-0.9940 +/- 0.0430
k4	-0.0988 +/- 0.0020	-0.1016 +/- 0.0027	-0.1017 +/- 0.0095	-0.1417 +/- 0.0357
k5	0.1841 +/- 0.0032	0.1598 +/- 0.0053	0.1781 +/- 0.0113	0.1638 +/- 0.0307
k6	0.0759 +/- 0.0014	0.0555 +/- 0.0037	0.0651 +/- 0.0064	0.0402 +/- 0.0226
k7	-0.0064 +/- 0.0025	0.0035 +/- 0.0052	0.0017 +/- 0.0113	0.0136 +/- 0.0266
k8	-0.0480 +/- 0.0028	-0.0356 +/- 0.0056	-0.0082 +/- 0.0103	0.0122 +/- 0.0277
	PHI = 0.6			
k1	-2.1848 +/- 0.0015	-1.8732 +/- 0.0023	-1.7458 +/- 0.0078	-1.7440 +/- 0.0177
k2	-0.5609 +/- 0.0023	2.8008 +/- 0.0036	3.0177 +/- 0.0198	3.1291 +/- 0.0361
k3	-1.3031 +/- 0.0026	-0.7189 +/- 0.0019	-0.6661 +/- 0.0106	-0.6312 +/- 0.0199
k4	-0.2267 +/- 0.0020	-0.1114 +/- 0.0021	-0.0901 +/- 0.0094	-0.0915 +/- 0.0077
k5	0.1295 +/- 0.0032	0.0641 +/- 0.0022	0.0599 +/- 0.0074	0.0966 +/- 0.0202
k6	0.0489 +/- 0.0016	0.0205 +/- 0.0025	0.0230 +/- 0.0045	0.0248 +/- 0.0065
k7	-0.0022 +/- 0.0021	-0.0041 +/- 0.0034	-0.0031 +/- 0.0068	0.0034 +/- 0.0215
k8	-0.0153 +/- 0.0028	-0.0091 +/- 0.0025	-0.0115 +/- 0.0066	0.0103 +/- 0.0200
	PHI = 0.8			
k1	-2.4734 +/- 0.0009	-1.4940 +/- 0.0012	-1.3354 +/- 0.0060	-1.3092 +/- 0.0139
k2	6.2960 +/- 0.0047	5.3562 +/- 0.0042	5.1857 +/- 0.0135	5.1752 +/- 0.0279
k3	-0.3673 +/- 0.0010	-0.3572 +/- 0.0012	-0.3471 +/- 0.0046	-0.3331 +/- 0.0144
k4	-0.0530 +/- 0.0007	-0.0548 +/- 0.0011	-0.0508 +/- 0.0024	-0.0456 +/- 0.0118
k5	0.0026 +/- 0.0013	0.0118 +/- 0.0015	0.0156 +/- 0.0029	0.0253 +/- 0.0078
k6	-0.0003 +/- 0.0010	0.0032 +/- 0.0012	0.0068 +/- 0.0034	0.0026 +/- 0.0074
k7	-0.0004 +/- 0.0008	0.0034 +/- 0.0014	-0.0032 +/- 0.0040	0.0012 +/- 0.0117
k8	0.0000 +/- 0.0010	-0.0016 +/- 0.0008	0.0000 +/- 0.0034	0.0059 +/- 0.0114
	PHI = 1.0			
k1	-0.8402 +/- 0.0003	-0.4545 +/- 0.0012	-0.3737 +/- 0.0037	-0.3705 +/- 0.0117
k2	10.4454 +/- 0.0015	6.9564 +/- 0.0029	6.4729 +/- 0.0081	6.3554 +/- 0.0348
k3	-0.0324 +/- 0.0003	-0.1471 +/- 0.0009	-0.1690 +/- 0.0027	-0.1756 +/- 0.0083
k4	-0.0024 +/- 0.0003	-0.0179 +/- 0.0011	-0.0248 +/- 0.0019	-0.0259 +/- 0.0048
k5	-0.0015 +/- 0.0003	0.0026 +/- 0.0007	0.0047 +/- 0.0019	0.0146 +/- 0.0045
k6	-0.0010 +/- 0.0001	0.0014 +/- 0.0006	-0.0005 +/- 0.0014	0.0069 +/- 0.0020
k7	-0.0009 +/- 0.0002	0.0008 +/- 0.0009	-0.0009 +/- 0.0019	0.0100 +/- 0.0036
k8	-0.0008 +/- 0.0002	-0.0004 +/- 0.0008	0.0004 +/- 0.0014	0.0089 +/- 0.0054

TABLE B-3-c: Taylor Coefficients, KAPPA = 18

	L = 2	L = 4	L = 8	L = 16
		PHI = 0.0		
k1	0.0017 +/- 0.0009	0.0015 +/- 0.0019	0.0047 +/- 0.0094	0.0019 +/- 0.0248
k2	8.0493 +/- 0.0216	-1.0759 +/- 0.0054	-1.1325 +/- 0.0287	-1.2518 +/- 0.0797
k3	-0.3056 +/- 0.0030	-0.8875 +/- 0.0037	-0.9320 +/- 0.0092	-0.9405 +/- 0.0244
k4	0.0414 +/- 0.0035	0.0386 +/- 0.0062	0.0229 +/- 0.0097	0.0595 +/- 0.0343
k5	0.0560 +/- 0.0029	0.2395 +/- 0.0079	0.2908 +/- 0.0130	0.3100 +/- 0.0265
k6	0.0319 +/- 0.0018	0.0631 +/- 0.0043	0.0747 +/- 0.0129	0.0578 +/- 0.0176
k7	-0.0024 +/- 0.0029	-0.0216 +/- 0.0031	-0.0191 +/- 0.0140	-0.0293 +/- 0.0138
k8	-0.0374 +/- 0.0025	-0.0828 +/- 0.0063	-0.0643 +/- 0.0202	-0.1106 +/- 0.0325
		PHI = 0.2		
k1	0.2052 +/- 0.0028	-0.7045 +/- 0.0033	-0.7401 +/- 0.0124	-0.7546 +/- 0.0146
k2	-4.9110 +/- 0.0082	-1.0499 +/- 0.0184	-1.1025 +/- 0.0292	-1.1341 +/- 0.0558
k3	-1.5820 +/- 0.0071	-0.9472 +/- 0.0052	-0.9828 +/- 0.0148	-0.9753 +/- 0.0381
k4	-0.0071 +/- 0.0091	0.0255 +/- 0.0042	0.0198 +/- 0.0152	0.0353 +/- 0.0430
k5	0.2633 +/- 0.0093	0.2294 +/- 0.0063	0.2505 +/- 0.0153	0.2552 +/- 0.0419
k6	0.1547 +/- 0.0050	0.0630 +/- 0.0039	0.0737 +/- 0.0129	0.0819 +/- 0.0275
k7	0.0054 +/- 0.0087	-0.0050 +/- 0.0045	-0.0088 +/- 0.0122	0.0429 +/- 0.0391
k8	-0.1354 +/- 0.0063	-0.0755 +/- 0.0042	-0.0638 +/- 0.0180	-0.0778 +/- 0.0457
		PHI = 0.4		
k1	-1.5374 +/- 0.0020	-1.4605 +/- 0.0026	-1.5032 +/- 0.0068	-1.5028 +/- 0.0139
k2	2.6551 +/- 0.0147	-0.4273 +/- 0.0080	-0.1508 +/- 0.0330	-0.0100 +/- 0.0606
k3	-0.7801 +/- 0.0064	-1.0715 +/- 0.0063	-1.0506 +/- 0.0123	-1.1186 +/- 0.0189
k4	-0.0111 +/- 0.0038	-0.0212 +/- 0.0045	-0.0169 +/- 0.0141	-0.0590 +/- 0.0324
k5	0.1343 +/- 0.0039	0.2155 +/- 0.0050	0.2397 +/- 0.0111	0.1867 +/- 0.0235
k6	0.0431 +/- 0.0037	0.0568 +/- 0.0043	0.0691 +/- 0.0100	0.0810 +/- 0.0194
k7	-0.0134 +/- 0.0047	-0.0081 +/- 0.0042	-0.0084 +/- 0.0116	0.0313 +/- 0.0305
k8	-0.0439 +/- 0.0048	-0.0598 +/- 0.0051	-0.0753 +/- 0.0147	-0.0241 +/- 0.0320
		PHI = 0.6		
k1	-1.4355 +/- 0.0016	-2.0901 +/- 0.0016	-2.0230 +/- 0.0090	-2.0050 +/- 0.0101
k2	-2.3451 +/- 0.0152	1.8690 +/- 0.0076	2.4576 +/- 0.0207	2.5062 +/- 0.0306
k3	-1.4753 +/- 0.0076	-1.0524 +/- 0.0052	-0.9645 +/- 0.0146	-0.9647 +/- 0.0176
k4	-0.1373 +/- 0.0046	-0.0948 +/- 0.0060	-0.0870 +/- 0.0102	-0.0588 +/- 0.0267
k5	0.2795 +/- 0.0115	0.1333 +/- 0.0054	0.1266 +/- 0.0106	0.1538 +/- 0.0308
k6	0.0868 +/- 0.0058	0.0443 +/- 0.0024	0.0184 +/- 0.0065	0.0593 +/- 0.0204
k7	-0.0228 +/- 0.0094	-0.0075 +/- 0.0039	-0.0076 +/- 0.0084	0.0272 +/- 0.0217
k8	-0.0483 +/- 0.0086	-0.0233 +/- 0.0060	-0.0021 +/- 0.0139	0.0214 +/- 0.0152
		PHI = 0.8		
k1	-3.6372 +/- 0.0021	-1.9930 +/- 0.0013	-1.7952 +/- 0.0066	-1.7597 +/- 0.0123
k2	4.8624 +/- 0.0146	6.0375 +/- 0.0082*	6.1368 +/- 0.0155	6.1811 +/- 0.0327
k3	-0.8718 +/- 0.0064	-0.6408 +/- 0.0044	-0.5913 +/- 0.0058	-0.5905 +/- 0.0128
k4	-0.1206 +/- 0.0037	-0.0860 +/- 0.0030	-0.0720 +/- 0.0083	-0.0957 +/- 0.0148
k5	0.0077 +/- 0.0034	0.0334 +/- 0.0028	0.0368 +/- 0.0056	0.0355 +/- 0.0111
k6	0.0057 +/- 0.0022	0.0113 +/- 0.0022	0.0089 +/- 0.0032	0.0068 +/- 0.0107
k7	0.0023 +/- 0.0040	0.0015 +/- 0.0022	-0.0082 +/- 0.0043	-0.0018 +/- 0.0075
k8	-0.0013 +/- 0.0031	-0.0037 +/- 0.0028	0.0060 +/- 0.0066	0.0114 +/- 0.0190
		PHI = 1.0		
k1	-1.4295 +/- 0.0009	-0.7670 +/- 0.0013	-0.6247 +/- 0.0045	-0.6030 +/- 0.0084
k2	16.0773 +/- 0.0088	9.5035 +/- 0.0032	8.8095 +/- 0.0130	8.6586 +/- 0.0156
k3	-0.0260 +/- 0.0007	-0.2487 +/- 0.0019	-0.2914 +/- 0.0051	-0.2892 +/- 0.0063
k4	-0.0033 +/- 0.0005	-0.0273 +/- 0.0014	-0.0320 +/- 0.0035	-0.0277 +/- 0.0078
k5	-0.0044 +/- 0.0005	0.0047 +/- 0.0012	0.0065 +/- 0.0035	0.0106 +/- 0.0084
k6	-0.0038 +/- 0.0004	0.0030 +/- 0.0014	0.0027 +/- 0.0029	0.0089 +/- 0.0053
k7	-0.0030 +/- 0.0008	0.0007 +/- 0.0010	0.0009 +/- 0.0035	-0.0003 +/- 0.0057
k8	-0.0043 +/- 0.0004	-0.0041 +/- 0.0015	0.0005 +/- 0.0038	-0.0009 +/- 0.0058

Appendix C: Supplement to Chapter IV

C.1. Decompositon of the φ^4 Hamiltonian into Terms with Different Dependence on the Fluctuation Field

The decomposition

$$\tilde{\mathcal{H}}(\bar{\psi}+\zeta) = \tilde{\mathcal{T}}_{\text{eff}}(\psi,\bar{\phi}) + \tilde{\mathcal{H}}(\zeta) + R(\psi|\zeta) \tag{1-1}$$

shall be performed for scalar φ^4 theory. We start from

$$\tilde{\mathcal{H}}(\varphi) = \frac{\tilde{\kappa}_0}{2}\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\varphi(z+\hat{\mu})-\varphi(z)]^2 + \frac{\tilde{m}_0^2}{2}\sum_{z\in\Lambda}\varphi(z)^2 + \frac{\tilde{\lambda}_0}{4!}\sum_{z\in\Lambda}\varphi(z)^4 \tag{1-2}$$

We set $\varphi \to \bar{\phi}+\zeta$ and consider separately the kinetic term, the mass term and the quartic interaction. We will use that because of the δ-function in the measure $\langle\cdot\rangle_\phi$ one can always substitute $\sum_{z\in x}\zeta(z) = L^d\bar{\phi}(x)$.

Split of the kinetic term:

$$\begin{aligned}
\sum_{z\in\Lambda}\sum_{\mu=1}^{d}\Big\{&[\bar{\psi}(z+\hat{\mu})-\bar{\psi}(z)]^2 + [\zeta(z+\hat{\mu})-\zeta(z)]^2 + 2[\bar{\psi}(z+\hat{\mu})-\bar{\psi}(z)][\zeta(z+\hat{\mu})-\zeta(z)]\Big\}\\
&- L^{d-1}\sum_{x\in\Lambda'}\sum_{\mu=1}^{d}[\psi(x+\hat{\mu}')-\psi(x)]^2\\
&+\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\zeta(z+\hat{\mu})-\zeta(z)]^2\\
&+2\sum_{x\in\Lambda'}\psi(x)\sum_{z\in x}(-\Delta\zeta)(z)
\end{aligned} \tag{1-3}$$

We have used that $\check{\psi}(z+\hat{\mu})-\check{\psi}(z)=0$ if z and $z+\hat{\mu}$ belong to the same block. If the link $(z, z+\hat{\mu})$ connects neighbouring blocks x and $x+\hat{\mu}'$ then $\check{\psi}(z+\hat{\mu})-\check{\psi}(z)=\psi(x+\hat{\mu}')-\psi(x)$. The factor L^{d-1} is due to the fact that the blocks x and $x+\hat{\mu}'$ are connected by L^{d-1} links. The last line of Eq. (1-3) is derived as follows:

$$\begin{aligned}
&\sum_{z\in\Lambda}\sum_{\mu=1}^{d}[\check{\psi}(z+\hat{\mu})-\check{\psi}(z)][\zeta(z+\hat{\mu})-\zeta(z)] \\
&\quad=\sum_{z\in\Lambda}\sum_{\mu=1}^{d}\check{\psi}(z)[2\zeta(z)-\zeta(z+\hat{\mu})-\zeta(z-\hat{\mu})] \\
&\quad=\sum_{z\in\Lambda}\check{\psi}(z)(-\Delta\zeta)(z) \\
&\quad=\sum_{x\in\Lambda'}\psi(x)\sum_{z\in x}(-\Delta\zeta)(z)
\end{aligned} \tag{1-4}$$

The contributions to the sum $\sum_{z\in x}(-\Delta\zeta)(z)$ cancel each other in the interior of the blocks. More precisely,

$$\sum_{z\in x}(-\Delta\zeta)(z)=-\sum_{\mu=\pm1}^{\pm d}\sum_{z\in\partial_\mu x}[\zeta(z+\hat{\mu})-\zeta(z)] \tag{1-5}$$

$\partial_\mu x$ is defined by

$$\partial_\mu x\equiv\{z\in x\,:\,z+\hat{\mu}\in x+\hat{\mu}'\} \tag{1-6}$$

Split of the mass term:

$$\begin{aligned}
&\sum_{z\in\Lambda}[\check{\psi}(z)^2+2\check{\psi}(z)\zeta(z)+\zeta(z)^2] \\
&\quad=L^d\sum_{x\in\Lambda'}\psi(x)^2 \\
&\quad+2L^d\sum_{x\in\Lambda'}\bar{\phi}(x)\psi(x) \\
&\quad+\sum_{z\in\Lambda}\zeta(z)^2
\end{aligned} \tag{1-7}$$

In free scalar field theory ($\lambda_0=0$) the term $\psi(x)\sum_{z\in x}[-\Delta\zeta](z)$ is the only coupling of block spin and fluctuation field. By a suitable splitting of the fundamental field φ into block spin and fluctuation part one can achieve that ϕ and ζ decouple in the free field field theory [17]. However, then the relation of fundamental field, fluctuation field and block spin is no longer strictly local. Therefore for our purpose the decomposition proposed in Chapter IV is more convenient.

Split of the interaction term:

$$\begin{aligned}
&\sum_{z\in\Lambda}[\check{\psi}(z)^4+4\check{\psi}(z)^3\zeta(z)+6\check{\psi}(z)^2\zeta(z)^2+4\check{\psi}(z)\zeta(z)^3+\zeta(z)^4] \\
&\quad=L^d\sum_{x\in\Lambda'}\psi(x)^4 \\
&\quad+4L^d\sum_{x\in\Lambda'}\bar{\phi}(x)\psi(x)^3 \\
&\quad+6\sum_{x\in\Lambda'}\psi(x)^2\sum_{z\in x}\zeta(z)^2 \\
&\quad+4\sum_{x\in\Lambda'}\psi(x)\sum_{z\in x}\zeta(z)^3 \\
&\quad+\sum_{z\in\Lambda}\zeta(z)^4
\end{aligned} \tag{1-8}$$

Putting things together one obtains

$$\begin{aligned}
&\tilde{\mathcal{H}}(\check{\psi}+\zeta)=\tilde{\mathcal{H}}(\zeta) \\
&\quad+\frac{\tilde{\kappa}_0}{2}\Big\{L^{d-1}\sum_{x\in\Lambda'}\sum_{\mu=1}^{d}[\psi(x+\hat{\mu}')-\psi(x)]^2+2\sum_{x\in\Lambda'}\psi(x)\sum_{z\in x}(-\Delta\zeta)(z)\Big\} \\
&\quad+\frac{\tilde{m}_0^2}{2}\Big\{L^d\sum_{x\in\Lambda'}[\psi(x)^2+2\bar{\phi}(x)\psi(x)]\Big\} \\
&\quad+\frac{\tilde{\lambda}_0}{4!}\Big\{L^d\sum_{x\in\Lambda'}[\psi(x)^4+4\bar{\phi}(x)\psi(x)^3]+6\sum_{x\in\Lambda'}\psi(x)^2\sum_{z\in x}\zeta(z)^2+4\sum_{x\in\Lambda'}\psi(x)\sum_{z\in x}\zeta(z)^3\Big\}
\end{aligned} \tag{1-9}$$

If one inserts the definitions of the rescaled coupling constants $\tilde{\kappa}_0$, $\tilde{m}_0^2$ and $\tilde{\lambda}_0$, for the part independent of ζ one finds

$$\begin{aligned}
\tilde{\mathcal{I}}_{\mathrm{eff}}(\psi|\bar{\phi})=\sum_{x\in\Lambda'}\Big\{&\frac{L}{2}\sum_{\mu=1}^{d}[\psi(x+\hat{\mu}')-\psi(x)]^2 \\
&+\frac{L^2m_0^2}{2}[\psi(x)^2+2\bar{\phi}(x)\psi(x)] \\
&+\frac{L^{4-d}\lambda_0}{4!}[\psi(x)^4+4\bar{\phi}(x)\psi(x)^3]\Big\}
\end{aligned} \tag{1-10}$$

The term which couples ζ and ψ is quadratic in ψ:

$$R(\psi|\zeta)=\sum_{x\in\Lambda'}\psi(x)\cdot\Xi_1(x|\zeta)+\sum_{x\in\Lambda'}\psi(x)^2\cdot\Xi_2(x|\zeta) \tag{1-11}$$

$\Xi_1(x|\zeta)$ and $\Xi_2(x|\zeta)$ are given by

$$\begin{aligned}\Xi_1(x|\zeta) &= \frac{L^{4-d}\lambda_0}{6} \operatorname*{av}_{z\in x} \zeta(z)^3 + L^2 \operatorname*{av}_{z\in x}(-\Delta\zeta)(z) \\ \Xi_2(x|\zeta) &= \frac{L^{4-d}\lambda_0}{4} \operatorname*{av}_{z\in x} \zeta(z)^2\end{aligned} \tag{1-12}$$

C.2. Expansion of Quadratic Lattice Functionals into a Series of Operators with Decreasing Perturbative Relevance

A procedure is described for a systematic expansion of translational invariant quadratic forms into a series of operators with decreasing perturbative relevance. The procedure in particular allows to extract a kinetic term from the quadratic Taylor coefficients of an effective Hamiltonian.

In the framework of perturbative renormalization group studies it is customary to expand effective Hamiltonians into interaction terms which are sums (integrals) of localized operators:

$$\mathcal{H}_{\text{eff}}(\underline{\phi}) = \sum_k g_k \int_x \mathcal{O}_x^{(k)}(\underline{\phi}) \tag{2-1}$$

$\int_x \equiv \sum_x a^d$. d is the dimension of the lattice, and a denotes the lattice spacing. In this appendix we consider fields $\underline{\phi}$ with dimension. They are related to the corresponding dimensionless fields ϕ by $\underline{\phi} = a^{\frac{1}{2}(2-d)}\phi$. The behaviour of an operator $\mathcal{O}_x^{(k)}(\underline{\phi})$ in perturbative renormalization group is determined essentially by its mass dimension R of its coupling constant g_k. The mass dimension D of the operator $\mathcal{O}_x^{(k)}(\underline{\phi})$ is made up from the canonical dimension of the involved fields $\underline{\phi}$ and the number of gradients: Each derivative increases the mass dimension by one. So, if the operator contains m fields and n gradients

$$D = m\left(\frac{d-2}{2}\right) + n \tag{2-2}$$

The degree of relevance R (= mass dimension of the coupling constant g_k) is given by $R = d - D$. Under a renormalization group transformation with scale factor L an operator scales (perturbatively) with a factor L^R. Operators with $R > 0$ ($R < 0$) are called relevant (irrelevant), such with $R = 0$ marginal.

Example: In $\underline{\phi}^4$ theory in four dimensions the kinetic term and the interaction term are marginal, the mass term is relevant.

Let us now consider quadratic functionals

$$(\underline{\phi}, h\underline{\phi}) \equiv \int_x \int_y \underline{\phi}(x) h(x,y) \underline{\phi}(y) \tag{2-3}$$

with a translationally invariant kernel $h(x,y) \equiv h(x-y)$.

$h(x) \equiv h(0,x)$ is assumed to be symmetric with respect to a permutation of the coordinates of x and with respect to reflections at the coordinate planes. We will assume that $\underline{\phi}$ is a scalar field. (Generalization to fields with several components is straightforward.) The functional $(\underline{\phi}, h\underline{\phi})$ shall be written in the form of Eq. (2-1). This can be achieved by Taylor expansion of one of the involved fields. Because of the translational invariance of h:

$$\begin{aligned}(\underline{\phi}, h\underline{\phi}) &= \int_x \int_y \underline{\phi}(x) h(x,y) \underline{\phi}(y) \\ &= \int_x \underline{\phi}(x) \int_y h(x, x+y) \underline{\phi}(x+y) \\ &= \int_x \underline{\phi}(x) \int_y h(y) \underline{\phi}(x+y)\end{aligned} \tag{2-4}$$

A systematic "Taylor expansion" of $\underline{\phi}(x+y)$ about x with the help of derivatives on the real space lattice is tedious. We will therefore use the momentum space representation where derivatives are represented by suitable multiplications.

$$\underline{\phi}(x+y) = \int_p e^{ipx}\, \tilde{\underline{\phi}}(p) \cdot e^{ipy} \tag{2-5}$$

$\int_p$ denotes the the integral over the first Brillouin zone: $\int_p \equiv \int_{-\pi/a}^{\pi/a} \frac{d^d p}{(2\pi)^d}$

$$(\underline{\phi}, h\underline{\phi}) = \int_x \underline{\phi}(x) \int_p e^{ipx}\, \tilde{\underline{\phi}}(p) \int_y h(y) e^{ipy} \tag{2-6}$$

We will use the lattice Laplacian Δ. (Because of the symmetry properties of the kernel h single derivatives do not occur.)

$$(\Delta f)(x) = a^{-2} \sum_{\mu=1}^{d} [f(x + a\hat{\mu}) + f(x - a\hat{\mu}) - 2f(x)] \equiv \int_y \Delta(x,y) f(y) \tag{2-7}$$

For the following it is convenient to define $a \equiv 1$. The Fourier representation of Δ is given by

$$\tilde{\Delta}(p) = \sum_{\mu=1}^{d} \tilde{\Delta}_\mu(p_\mu) \tag{2-8}$$

Multiplication (in momentum space) with $\tilde{\Delta}_\mu$ corresponds to 2-fold differentiation in μ-direction (in real space).

$$\tilde{\Delta}_\mu(p_\mu) = e^{ip_\mu} + e^{-ip_\mu} - 2 = 2\cos p_\mu - 2 = -4\sin^2 \frac{p_\mu}{2} \tag{2-9}$$

The relation of $\tilde{\Delta}_\mu(p_\mu)$ and p_μ^2 can be inverted:

$$p_\mu^2 = 4 \arcsin^2 \sqrt{\frac{-\tilde{\Delta}_\mu(p_\mu)}{4}} \tag{2-10}$$

$\arcsin^2$ has a power series representation (see e.g. [46])

$$\arcsin^2 x = \sum_{k=0}^{\infty} \frac{2^{2k} k!}{(2k+1)!(k+1)} \cdot (x^2)^{k+1} \tag{2-11}$$

which converges for $x^2 \leq 1$. We thus find

$$\begin{aligned} p_\mu^2 &= \sum_{k=0}^{\infty} \frac{k!}{(2k+1)!(k+1)} \cdot [-\tilde{\Delta}_\mu(p_\mu)]^{k+1} \\ &= [-\tilde{\Delta}_\mu(p_\mu)] + \frac{1}{12}[-\tilde{\Delta}_\mu(p_\mu)]^2 + \frac{1}{180}[-\tilde{\Delta}_\mu(p_\mu)]^3 + \cdots \end{aligned} \tag{2-12}$$

Let us now return to Eq. (2-6).

$$\begin{aligned} \int_y h(y) e^{ipy} &= \int_y h(y) \cos(py) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \int_y h(y) (py)^{2n} \end{aligned} \tag{2-13}$$

The decompositon of the power of the scalar product py is

$$(py)^{2n} = (p_\mu y_\mu)^{2n} = p_{\mu_1} \cdots p_{\mu_{2n}} \cdot y_{\mu_1} \cdots y_{\mu_{2n}} \tag{2-14}$$

Summation over repeated indices is understood. We now define moments

$$h_{\mu_1 \ldots \mu_{2n}} \equiv \int_y h(y)\, y_{\mu_1} \ldots y_{\mu_{2n}} \tag{2-15}$$

The quadratic form $(\underline{\phi}, h\, \underline{\phi})$ thus has a representation

$$(\underline{\phi}, h\, \underline{\phi}) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \int_x \underline{\phi}(x) \int_p e^{ipx} \tilde{\underline{\phi}}(p)\, p_{\mu_1} \cdots p_{\mu_{2n}}\, h_{\mu_1 \ldots \mu_{2n}} \tag{2-16}$$

We determine the coefficients of the expansion for $n \leq 2$. Taking advantage of the symmetry properties of h one finds

$$\begin{aligned} p_\alpha p_\beta \cdot h_{\alpha\beta} &= \sum_\alpha p_\alpha^2\, h_{\alpha\alpha} = h_{11} \sum_\alpha p_\alpha^2 \\ &= h_{11}[(-\tilde{\Delta}) + \frac{1}{12} \sum_\alpha \tilde{\Delta}_\alpha^2] + O(\tilde{\Delta}^3) \end{aligned} \tag{2-17}$$

$$\begin{aligned} p_\alpha p_\beta p_\gamma p_\delta \cdot h_{\alpha\beta\gamma\delta} &= (h_{1111} - 3h_{1122}) \sum_\alpha p_\alpha^2 p_\alpha^2 + h_{1122} (\sum_\alpha p_\alpha^2)^2 \\ &= (h_{1111} - 3h_{1122}) \sum_\alpha \tilde{\Delta}_\alpha^2 + h_{1122}\, \tilde{\Delta}^2 + O(\tilde{\Delta}^3) \end{aligned} \tag{2-18}$$

Thus the result is

$$(\underline{\phi}, h\, \underline{\phi}) = g_1 \int \underline{\phi}^2 + g_2 \int \underline{\phi} \Delta \underline{\phi} + g_3 \int \underline{\phi} [\sum_\alpha \Delta_\alpha^2] \underline{\phi} + g_4 \int \underline{\phi} \Delta^2 \underline{\phi} + O(\Delta^3) \tag{2-19}$$

with coefficients

$$\begin{aligned} g_1 &= h_0 = \int_y h(y) \\ g_2 &= \frac{1}{2} h_{11} = \frac{1}{2d} \int_y h(y)\, y^2 \\ g_3 &= -\frac{1}{24} h_{11} + \frac{1}{24}(h_{1111} - 3h_{1122}) \\ g_4 &= \frac{1}{24} h_{1122} \end{aligned} \tag{2-20}$$

In four dimensions g_1 is a relevant coupling, g_2 is marginal (kinetic term), g_3 and g_4 are irrelevant.

−4	1
1	

20	−8	1
−8	2	
1		

−112	57	−12	1
57	−24	3	
−12	3		
1			

676	−400	112	−16	1
−400	216	−48	4	
112	−48	6		
−16	4			
1				

The nonvanishing matrix elements of $\Delta^n(0,x) \equiv \Delta^n(x)$, $n \leq 4$, for a 2-dimensional lattice. The numbers were obtained by Fourier transformation of $\tilde{\Delta}(p)$. The values are given only in one of the four sectors of the lattice.

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