Critical Phenomena with Linked Cluster Expansions in a Finite Volume

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Abstract
Linked cluster expansions are generalized from an infinite to a finite volume. They are performed to 20th order in the expansion parameter to approach the critical region from the symmetric phase. A new criterion is proposed to distinguish 1st from 2nd order transitions within a finite size scaling analysis. The criterion applies also to other methods for investigating the phase structure such as Monte Carlo simulations. Our computational tools are illustrated at the example of scalar $O(N)$ models with four and six-point couplings for $N = 1$ and $N = 4$ in three dimensions. It is shown how to localize the tricritical line in these models. We indicate some further applications of our methods to the electroweak transition as well as to models for superconductivity.

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1 Introduction

The phase structure of models for strong and electroweak interactions has been a topic of intensive research in the past. In spite of numerous investigations some central questions are still open. To these belong the nature of the chiral/deconfinement transition in QCD for physical values of the current quark masses and the strength of the electroweak transition for the physical (so far unknown) Higgs mass. In both realms one has to account for nonperturbative coupling regions. Thus it is natural to choose the lattice regularized version of these theories to study their phase structure. Most applications are performed with Monte Carlo simulations, which are an appropriate tool to study the critical region. Monte Carlo simulations are restricted to a finite volume. Thorough extrapolations to the infinite volume limit from a finite size scaling analysis is in general expensive and sometimes impracticable for lattice sizes which are realistic for QCD or for the standard model [1].

Convergent expansions such as Linked Cluster or Hopping Parameter Expansions (HPEs) provide an analytic alternative to Monte Carlo simulations. They may also serve as a convenient supplement to numerical calculations. Originally they have been developed in the \textit{infinite} volume. In contrast to generic perturbation theory about noninteracting fields, HPEs are convergent power series expansions about completely disordered lattice systems. Under certain conditions their convergence radius can be directly related to the location of the physical singularity. Hence, similarly to Monte Carlo simulations, HPEs can be applied to the phase transition (critical) region, if the order in the hopping parameter \( \kappa \) is just high enough. Thus the transition region is accessible from the high temperature (symmetric) phase.

Hopping parameter expansions have a long tradition in statistical physics ([2, 3, 4] and references therein). Their generalization and application to particle physics have been pioneered by Lüscher and Weisz [5]. Lüscher and Weisz studied a lattice \( \Phi^4 \)-theory close to its continuum limit in four dimensions [3, 4]. Recently, the HPE has been generalized to field theories at finite temperature [8]. The generalization is twofold. First of all one has to implement a toroidal symmetry in one direction of finite extension, say \( L_0 \). In this context the temperature \( T \) is given by \( T = L_0^{-1} \) in lattice units. Second, the highest computed order in the expansion parameter has to be increased, because the toroidal (temperature) effect on the critical coupling is rather small. Typically, the critical hopping parameter \( \kappa_c \) changes only by a few percent even on a \( 4 \times \infty^3 \) lattice compared to the \( \infty^4 \) lattice. The graphs of the expansion can only "feel the temperature", if they are able to wind around the torus in the temperature direction. In general, the largest possible winding number should be larger than one to induce a measurable effect. In [8] the 18th order has been used to determine the critical behaviour of the finite temperature \( \Phi^4 \) models with O(N) symmetry. Meanwhile, the 20th order of this expansion is available for 2-point susceptibilities, see below.

In this paper we extend the HPE to a finite volume, i.e. to a lattice with toroidal symmetry in all directions. We propose criteria to distinguish first from second order
transitions (and crossover phenomena) both in an infinite and in a finite volume. It is the fate of power series expansions that one cannot work at the singularity \( \kappa_c \), one can only come close to it, the closer, the higher the order in the expansion. Thus we need a criterion that works slightly below \( \kappa_c \). As such a criterion we propose a so called monotony criterion which is based on the specific volume dependence of truncated correlation functions close to but not at the transition point. The criterion includes both order parameter susceptibilities and other singular response functions such as the specific heat. Decrease or increase with the volume identifies first or second order transitions, respectively. Although the monotony criterion has been developed in the framework of HPEs, it is not restricted to this case. It can be used in other methods as well, in particular in Monte Carlo simulations.

As a second application of the HPE in a finite volume we calculate an effective potential up to 16th order in the hopping parameter. The shape of the effective potential further characterizes the type of transition. The coexistence of distinct minima at the critical point provides another possibility to calculate \( \kappa_c \) in a finite volume.

The criteria will be applied to scalar \( O(N) \)-models with \( \Phi^4 \) and \( \Phi^6 \) self-interactions in three dimensions. These models allow for various first and second order transition regions in the bare coupling constant space. For fixed couplings the phase transitions will be considered as a function of \( \kappa \). The parameter \( \kappa \) may be identified with an inverse temperature \( 1/T \) of a classical system with the same action in three dimensions. Thus we will sometimes replace \( \kappa_c \) by \( T^{-1}_c \). In connection with a field theory in four spacetime dimensions the three dimensional model may be considered as an effective description of the four dimensional model at finite temperature, arising in a process of dimensional reduction. In a four dimensional theory at finite temperature one should distinguish between \( \kappa \) and \( T^{-1} \).

The scalar \( O(N) \)-models contain a number of interesting special cases. If the four-and six-point couplings are sent to infinity in an approriate way, we obtain "diluted" \( O(N) \) models, i.e. Heisenberg models with additional occupation number variables, for \( N = 1 \) we have a diluted Ising model. The case of \( N = 4 \) and pure quartic selfinteraction is assumed to share the universality class with QCD in the limit of two massless flavours. It also corresponds to the scalar sector of the electroweak standard model. A \( \Phi^4 + \Phi^6 \)-theory exhibits a tricritical point (line) for a fixed (varying) six-point coupling. Such a tricritical point is observed in a liquid mixture of \( He^3/He^4 \). Recently it has been also proposed as candidate for representing the universality class of tricritical QCD \([10, 11]\). (Tricritical QCD means QCD with vanishing up and down quark masses and a strange quark mass which takes a critical value, at which the chiral transition changes its order.) We indicate how to localize the tricritical line in a \( \Phi^4 + \Phi^6 \)-theory with our methods.

The outline of the paper is as follows. In section 2.1 we summarize the main results for HPEs from \([8]\). It basically serves to fix the notation. We then extend the HPE in an infinite volume to a graphical expansion in a finite volume (section 2.2). In section 3 we give two criteria to distinguish 1st from 2nd order transitions: a
precise formulation of the monotony criterion (section 3.1), and an effective potential evaluated in the HPE in a finite volume (section 3.2). In section 4 we apply these criteria to three-dimensional scalar $O(N)$ models with renormalizable interactions. To get a first estimate on the phase structure in bare coupling parameter space, we study the large coupling limit by a saddle point integration. Another estimate for the location at finite couplings is obtained from a hopping-mean-field analysis. This approximation amounts to a tree level evaluation of the HPE (Section 4.1). After this preliminary study of the phase structure we present a more detailed investigation by means of the HPE. In the infinite volume limit, plateaus of critical exponents as obtained from the linked cluster series are proposed as criteria to identify the various universality classes of the critical region of the theory (Section 4.2). In Section 4.3 we discuss the finite volume behaviour of various quantities. The shift in volume of the critical coupling $\kappa_c$, defined here as the radius of convergence, is compared to the scaling behaviour which is expected for the shift of the maximum of the order parameter susceptibility. The monotony criterion and the effective potential are evaluated for points both in the first and second order coupling region. Finally we show how to locate the tricritical line. In section 5 we summarize our results and give an outlook to further physical applications.

2 Hopping parameter expansions for the critical region

2.1 General framework

Linked cluster expansions provide a convenient tool for both numerical and analytic studies of lattice field theories. The typical expansion parameters are the coupling strengths between fields at different lattice sites [2, 3]. In contrast to saddle point expansions which are at most asymptotically convergent, series resulting from HPE are absolutely convergent for sufficiently small couplings [12]. In this sense they can be viewed as generalized high temperature expansions. If in addition the sign of susceptibility series is uniform, the radius of convergence identifies the phase transition, i.e. the critical temperature.

In order to extract quantitative information on the critical behaviour one has to get sufficiently close to the critical point. The price to be paid is a computation to high orders. The realization of such expansions by convenient algorithms with the aid of computers has been pioneered by Lüscher and Weisz [5]. Recently, progress in various ways has been made to extend the length of strong coupling series [8, 13, 14]. Normally, these expansions are set up in an infinite volume. In [8], the techniques have been further developed in such a way that the expansions can be reliably applied to lattices of non-trivial topology. In particular, it turned out that the highest order in the expansion had to be further increased for measuring effects from topology. The improved techniques have been applied to scalar $O(N)$ models with quartic
interaction on 4-dimensional finite temperature lattices \([9]\). The critical exponents could be shown to agree with the critical indices of the corresponding (dimensionally reduced) 3-dimensional models.

In the following we summarize the main formulas from \([5, 8]\) to fix the notation and to set up the expansion scheme that later will be generalized to a finite volume. We consider a \(D\)-dimensional hypercubic lattice \(\Lambda = \times_{i=0}^{D-1} \mathbb{Z} / L_i\), with \(L_i \in \mathbb{N}\) an even number or with \(L_i = \infty\). Periodic boundary conditions are imposed for each finite \(L_i\). The restriction to even \(L_i\) leads to a considerable reduction of the number of contributing graphs because it implies that each loop must have an even number of lines. The class of models we discuss are described by the partition function

\[
Z(J, v) = \int \prod_{x \in \Lambda} d^N \Phi(x) \exp \left( \frac{1}{2} \sum_{x \neq y \in \Lambda} \sum_{a, b=1}^N \Phi_a(x)v_{ab}(x, y)\Phi_b(y) \right) \\
\cdot \exp \left( -\sum_x S(\Phi(x)) + \sum_{x \in \Lambda} \sum_{a=1}^N J_a(x)\Phi_a(x) \right),
\]

(1)

where \(\Phi\) denotes a real, \(N\)-component scalar field, \(J\) are external sources, \(v_{ab}(x, y)\) denote the hopping couplings. The ultralocal part of the action \(S\), which depends only on one lattice site, is chosen to be \(O(N)\) invariant. It should guarantee the stability of the partition function \([1]\) for sufficiently small \(v(x, y)\). Throughout this paper we consider as an example the action of a \(\Phi^4 + \Phi^6\)-theory

\[
S(\Phi) = \Phi^2 + \lambda(\Phi^2 - 1)^2 + \sigma(\Phi^2 - 1)^3,
\]

(2)

which exhibits a phase structure with both first and second order transitions. We emphasize, however, that the general techniques are not restricted to this case.

Fields at different lattice sites interact with the hopping coupling \(v_{ab}(x, y)\). For the case of nearest neighbour interactions, it reduces to

\[
v_{ab}(x, y) = \begin{cases} 
2\kappa \delta_{a,b} & , \ \text{x, y nearest neighbour} \\
0 & , \ \text{otherwise,}
\end{cases}
\]

(3)

where \(\kappa\) is the so called hopping parameter. The nearest neighbour property should be understood modulo the torus lengths. Henceforth we consider only nearest neighbour interactions.

The generating functional of connected correlation functions is given by

\[
W(J, v) = \ln Z(J, v), \\
W^{(2n)}_{a_1 \ldots a_{2n}}(x_1, \ldots, x_{2n}) = \left< \Phi_{a_1}(x_1) \cdots \Phi_{a_{2n}}(x_{2n}) \right>^c \]

\[
\frac{\partial^{2n}}{\partial J_{a_1}(x_1) \cdots \partial J_{a_{2n}}(x_{2n})} W(J, v) \bigg|_{J=0}.
\]

(4)
In the following a major role is played by the connected 2-point function and the corresponding susceptibility $\chi_2$ and moments $\mu_2$, defined according to

$$\delta_{a,b} \chi_2 = \sum_x < \Phi_a(x)\Phi_b(0) >^c,$$

$$\delta_{a,b} \mu_2 = \sum_x \left( \sum_{i=0}^{D-1} x_i^2 \right) < \Phi_a(x)\Phi_b(0) >^c.$$

In field theory, it is convenient to define the renormalized coupling constants via the vertex functional

$$\Gamma(M) = W(J) - \sum_{x \in \Lambda} J(x) \cdot M(x)$$

$$= \sum_{n \geq 0} \frac{1}{2n!} \sum_{a_1, \ldots, a_{2n}} \Gamma_{a_1 \ldots a_{2n}}^{(2n)}(x_1, \ldots, x_{2n}) M_{a_1}(x_1) \cdots M_{a_{2n}}(x_{2n}),$$

$$M_a(x) = \frac{\partial W}{\partial J_a(x)}, \quad a = 1, \ldots, n.$$

The standard definitions of the renormalized mass $m_R$ (as inverse correlation length) and the wave function renormalization constant $Z_R$ are

$$\tilde{\Gamma}_{a b}^{(2)}(p, -p) = -\frac{1}{Z_R} (m_R^2 + p^2 + O(p^4)) \delta_{a,b} \quad \text{as} \quad p \to 0,$$

where $\tilde{\cdot}$ denotes the Fourier transform. Eq. (7) implies that

$$m_R^2 = 2D \frac{\chi_2}{\mu_2}, \quad Z_R = 2D \frac{\chi_2^2}{\mu_2}.$$

The critical exponents $\gamma, \nu, \eta$ are defined by the leading singular behaviour at the critical point $\kappa_c$,

$$\ln \chi_2 \simeq -\gamma \ln (\kappa_c - \kappa),$$

$$\ln m_R^2 \simeq 2\nu \ln (\kappa_c - \kappa), \quad \text{as} \quad \kappa \searrow \kappa_c,$$

$$\ln Z_R \simeq \nu \eta \ln (\kappa_c - \kappa),$$

such that $\nu \eta = 2\nu - \gamma$.

If the interaction part (3) of the action is switched off, i.e. $v = 0$, $S(\Phi, v = 0) = \sum_x \tilde{S}(\Phi(x))$, the partition function factorizes, and in turn $W(J, v = 0) = \sum_x W(J(x))$. In particular,

$$W_{a_1 \ldots a_{2n}}^{(2n)}(x_1, \ldots, x_{2n}) = \begin{cases} \frac{\delta_{a_1 \ldots a_{2n}}^{c}(x_1, \ldots, x_{2n})}{(2n-1)!!} C_{2n}(a_1, \ldots, a_{2n}) & \text{for } x_1 = x_2 = \cdots = x_{2n} \\ 0 & \text{otherwise} \end{cases}$$

(10)
with
\[ v_{2n}^c = \frac{\partial^{2n}}{\partial J_{1}^{2n}} W(J) \bigg|_{J=0}, \]  
and \( C_{2n} \) totally symmetric coefficients in \( a_i, i = 1...2n \).

In practice, the vertex couplings \( v_{2n}^c \) are obtained from the relation
\[
\bar{W}(J) = \sum_{n \geq 1} \frac{1}{(2n)!} v_{2n}^c (J^2)^n
\]
\[
= \ln \left( 1 + \sum_{n \geq 1} \frac{1}{(2n)!} v_{2n}^c (J^2)^n \right),
\]
with
\[
\bar{v}_{2n} = \frac{\int d^N \Phi \Phi^{2n} \exp \left( -\bar{S} (\Phi) \right)}{\int d^N \Phi \exp \left( -\bar{S} (\Phi) \right)},
\]
or, alternatively, recursively from Dyson-Schwinger equations.

The linked cluster expansion for \( W \) is the Taylor expansion with respect to \( v(x, y) \) about this decoupled case,
\[
W(J, \hat{v}) = \left( \exp \sum_{x,y} \sum_{a,b} v_{ab}(x, y) \frac{\partial}{\partial v_{ab}(x, y)} \right) W(J, \hat{v}) \bigg|_{\hat{v}=0}.
\]

The corresponding expansions of correlation functions are obtained from (14) by (4). Susceptibilities become power series in \( \kappa \) with a nonvanishing radius of convergence.

The management of such an expansion is conveniently done by means of a graph theoretical device. Correlation functions are represented as a sum over equivalence classes of graphs, each class being endowed with an appropriate weight. In order to make high orders in the expansion feasible it is necessary to introduce more restricted subclasses of graphs such as 1-particle irreducible (1PI) graphs, 1-vertex irreducible graphs, and renormalized moments. The correlations are then represented in terms of the latter two. For further details we refer to [5, 8].

The weight of each graph decomposes into a product of its (inverse) symmetry number, the \( \text{O(N)} \)-group factor, and the lattice embedding number. It is only the latter one that depends on the topology of the particular lattice which is involved. In the next section we outline the modifications of the embedding numbers due to a finite volume.

### 2.2 Extension to the torus

Let us consider a correlation function, such as in (5), on a \( D \)-dimensional lattice of size \( L_0 \times L_1 \times ... \times L_{D-1} \) with periodic boundary conditions. Except for a trivial volume factor, the embedding number \( I_{\Gamma}(L_0, \ldots, L_{D-1}) \) of a connected graph \( \Gamma \) counts the number of possible ways \( \Gamma \) can be embedded on the lattice. Embedding
means a mapping of every vertex $v$ of $\Gamma$ onto a lattice site $x(v) = (x_0, \ldots, x_{D-1})(v)$ consistent with the topology of $\Gamma$. Every two vertices have to be mapped to nearest neighbour lattice sites if they are neighboured vertices of $\Gamma$, i.e. if they are connected by at least one line. Selflines do not exist. Otherwise the linked cluster expansion does not impose any exclusion constraints. In particular, an arbitrary number of vertices can occupy the same lattice site.

It is most convenient to rearrange the computation of embedding numbers in terms of random walks [13]. Towards this end, the set of vertices of $\Gamma$ is divided into the disjoint sets of internal 2-vertices and their complement. A vertex $v$ is called internal 2-vertex, if it has no external line attached, and there are precisely two neighboured vertices of $v$ in $\Gamma$. All internal 2-vertices can be reorganized into so-called 2-chains between the remaining vertices in an obvious way. Every 2-chain $c$ has an initial vertex $i_c$ and a final vertex $f_c$, possibly identical, and it has a length $l_c \geq 1$, where $l_c - 1$ denotes the number of internal 2-vertices of $c$. Here, for convenience, we include $l_c = 1$, in which case $c$ just implies the nearest neighbour constraint on $i_c$ and $f_c$. On the lattice infinite in all directions the embedding number is then written as

$$I_{\Gamma}(\infty^D) = \sum_{(x(v))} \prod_c N_{x(i_c) \rightarrow x(f_c)}^{l_c,D}(\infty^D).$$

The sum runs over all placements of vertices $v$ that are not internal 2-vertices, with $x(v_0)$ kept fixed for some arbitrary vertex $v_0$ to account for the trivial entropy factor. The product runs over all 2-chains of $\Gamma$. $N_{x \rightarrow y}^{l,D}(\infty^D)$ denotes the number of free random walks of length $l$ from lattice site $x$ to $y$. Closed analytic expressions can be given for $N_{x \rightarrow y}^{l,D}$. We notice that

$$N_{x \rightarrow y}^{l,D}(\infty^D) \neq 0 \text{ only if } l - \sum_{i=0}^{D-1} |x_i - y_i| \geq 0 \text{ even.} \quad (16)$$

In the finite volume with periodic boundary conditions the topology modifies [13] at two places. First, the sites $x(v)$ are now restricted to a cube of size $L_0 \times L_1 \times \ldots \times L_{D-1}$, and the nearest neighbour constraint, implicit in every 2-chain $c$ of length $l_c = 1$ holds modulo the torus lengths. Second, the number of random walks $N_{x \rightarrow y}^{l_c,D}(\infty^D)$ is replaced by

$$N_{x \rightarrow y}^{l_c,D}(L_0, \ldots, L_{D-1}) = \sum_{\mu_0, \ldots, \mu_{D-1} \in \mathbb{Z}} N_{x \rightarrow y + \mu \cdot L}^{l_c,D}(\infty^D), \quad (17)$$

where

$$\mu \cdot L = \sum_{i=0}^{D-1} \mu_i L_i.$$

The sum in (17) accounts for additional random walks which arise from the possible winding around the torus. Due to (16), the sum in (17) is finite.
3 Finite size scaling analysis with HPE

In this section we discuss two criteria in the finite volume to determine the order of a phase transition. Although the criteria are developed for linked cluster expansions, their application is not restricted to series representations.

The question arises, why one is interested in linked cluster expansion on a torus, since the expansion are more easily obtained in the infinite volume. Data of the critical region such as the critical temperature are successfully extracted from the asymptotic high order behaviour of the coefficients of susceptibility series. The typical precision here is within 4-5 digits or even better.

In general the symmetry of the model alone does not determine the properties of a transition. For instance, there may be more than one universality class, corresponding to different ranges in the space of bare actions. As was pointed out in [9], one should look for plateaus of critical exponents to distinguish between them. Problems arise close to the boundary of two such domains. ”Smearing effects” occur due to the truncation of the series. Both universality domains will influence the coefficients, the more the lower the order. This does not pose a problem, as long as the domains are sufficiently large and the boundary of the domains extends over a negligible coupling range.

Whereas the location of the phase transition can be determined very precisely from the infinite volume series, its order is usually a more intricate question, in particular, if the transition is weakly first order. Criteria to distinguish 1st and 2nd order transitions can be conveniently worked out in the finite volume. Thus, in our case, the finite size effects will be utilized rather than suppressed as artifacts of the finite volume.

A finite size scaling analysis for second order transitions can be based on a renormalization group approach, see e.g. [15]. The inverse linear size $L^{-1}$ of the system is put on an equal footing with other scaling fields like the temperature or an external field. The analysis results in a prediction of the leading scaling behaviour of a susceptibility $\chi$ about the critical temperature $T_c$ according to

$$\chi(t, L) \simeq |t|^{-\gamma} P(L/\xi_\infty(t))$$

for sufficiently small $t$ and large $L$, where $t$ is the reduced temperature $(T - T_c)/T_c$, and $\gamma$ is the critical exponent characterizing the divergence at $t = 0$. The amplitude $P$ depends only on $L$ measured in units of the infinite volume correlation length $\xi_\infty$.

Further properties of $P$ ensure that the height of the peak of the susceptibility at $T_c(L)$ scales according to $\chi(T_c(L), L) \simeq L^{(\gamma/\nu)}$, the width $\sigma(L)$ of the critical region shrinks with $L^{-1/\nu}$, and $T_c(L)$ is shifted compared to $T_c$ according to $T_c(L) - T_c \simeq L^{-1/\nu}$. Here $\nu$ denotes the critical exponent of the correlation length.

For a generic first order transition an analogous derivation of the scaling behaviour from first principles is missing in general. The ratio $L/\xi_\infty(t)$ is no longer a distinguished scaling variable. In the thermodynamic limit, as $T$ approaches $T_c$, the
correlation stays finite and model dependent. The rounding and shifting of thermodynamic singularities are normally described in a phenomenological approach \[16\] which is based on Monte Carlo results. The height of the peak of the susceptibility at \( T_c(L) \) is expected to scale with \( L^D \), both the width \( \sigma(L) \) and the shift in \( T_c(L) - T_c \) are expected to scale with \( L^{-D} \) as \( L \to \infty \), where \( D \) denotes the space(time) dimension. A more fundamental finite size scaling theory exists for a class of spin models that allow for a particular polymer expansion of the partition function \[17\]. Whereas the predictions of the finite size scaling of the height of the peak and the width of the scaling region reproduce the above mentioned behaviour, the shift of the location of the peak is derived to be \( T_c(L) - T_c \simeq L^{-2D} \).

It turns out that our series representations in the hopping parameter \( \kappa \) for the susceptibilities \( \chi \) cannot be uniquely extrapolated to the critical \( \kappa_c \) (corresponding to \( T_c^{-1} \) as explained in the introduction) to the end that the peak and width of \( \chi \) confirm the expected scaling behaviour. However, the specific behaviour of \( \chi \) close to \( \kappa_c \) is conclusive enough for distinguishing regions of 1st and 2nd order transitions, as we will show below, without any need for an extrapolation in \( \kappa \) to \( \kappa_c \). In addition, the scaling of \( \kappa_c(L) \), defined as the radius of convergence in the finite volume, follows the form expected (by analogy) for the shift of the location of the peak from \[17\]. The scaling behaviour holds for the \( \mathbb{Z}_2 \) model, but also for the \( \Phi^4 + \Phi^6 \)-models with four components, which are not covered by the analysis of \[17\], cf. section IV.3.

### 3.1 The monotony criterion

For a certain interval of the scaling region response functions with a nonanalytic behaviour in the infinite volume limit show different monotony behaviour for 1st and 2nd order transitions. Examples for such functions are the specific heat and order parameter susceptibilities. They are increasing in volume in a certain neighbourhood of \( T_c \) for 2nd order transitions, and decreasing for 1st order transitions for some range in the scaling region, which will be specified below. Since we are not aware of any discussion in the literature, although the underlying idea is rather simple, we will describe the behaviour in some detail. For definiteness we fix the notation in terms of order parameter susceptibilities.

From the standard finite size scaling analysis one knows that

\[
\chi(t, L = \infty) < \infty \quad \text{as} \quad t \to 0
\]

for a 1st order transition with a possible discontinuity, whereas

\[
\chi(t, L = \infty) \simeq \mathcal{A}|t|^{-\gamma}
\]

for a 2nd order transition with critical exponent \( \gamma > 0 \). By definition, regular contributions to \( \chi \) may be neglected in the scaling region. On the other hand, \( \chi(0, L) \) diverges in both cases as \( L \) approaches infinity. More precisely, at \( T_c \), \( \chi \) has a "\( \delta \)-function" or power law type of singularity for a 1st or 2nd order transition in
the thermodynamic limit, respectively. It is this difference that is responsible for the different monotony properties for \( t \neq 0 \) in the finite volume. If \( t \neq 0 \) is small, to a given lattice size \( L_s < \infty \), not too small, one can always find a second size \( L_l \) with \( L_l > L_s \) such that

\[
\chi(t, L \geq L_l) > \chi(t, L_s) \quad \text{for 2nd order,} \tag{21}
\]

\[
\chi(t, L \geq L_l) < \chi(t, L_s) \quad \text{for 1st order,} \tag{22}
\]

that is, \( \chi \) is increasing or decreasing in volume. In the series representation of \( \chi \) we can set \( L_l = \infty \), so that (21) and (22) give strong criteria in the whole scaling region where we can use the series. If the volume cannot be made infinite, as in Monte Carlo simulations, one is confined to \( L \leq L_0 \) for some \( L_0 \). Eq. (22) then still holds except for a small neighbourhood of \( T_c \), where the susceptibility is increasing in volume as in the 2nd order case. The width of this neighbourhood is rapidly decreasing with increasing \( L_0 \).

In the following we make these statements more precise. Let \( t \) denote the scaling field, i.e. \( t = (T - T_c)/T_c \), \( v \) the inverse volume or an appropriate power of it. The infinite volume limit is obtained as \( v \to 0 \) from above. The transition range is then given by small \( t \) and \( v \). Let

\[
H^2 := \{(t, v) \in \mathbb{R}^2 \mid v \geq 0\}
\]

(23)

denote a half plane, \( \mathcal{U} \subseteq H^2 \) an open neighbourhood of \( 0 \in H^2 \) and \( \mathcal{U}^* = \mathcal{U} \setminus \{0\} \).

We discuss the case of a first order transition first. The typical behaviour of a susceptibility close to the transition is described by the following

**Definition 3.1** For any \( \omega > 0 \) we define \( \Psi_\omega(\mathcal{U}) \) as the set of real valued continuous functions \( \chi : \mathcal{U}^* \to \mathbb{R} \) with the following properties.

1. \( \chi \in C^1(\mathcal{U}^* \setminus \{(\mathbb{R}, 0)\}) \), that is, \( \chi \) is once continuously differentiable for \( v \neq 0 \).
2. For all nonzero \( t \) there is \( \nu_t > 0 \) such that for all \( v < |t|/\nu_t \)

\[
| \chi(t, v) | \leq \omega.
\]

3. With appropriate positive constants \( c, K_1, K_2 \) and \( \epsilon \) we have in \( \mathcal{U}^* \) for \( v \neq 0 \)

\[
| \chi(0, v) - c/v | < \frac{K_1}{v^{1-\epsilon}},
\]

\[
| \frac{\partial}{\partial t} \chi(t, v) | < \frac{K_2}{v^2}.
\]

As an example, consider the following representation of the magnetic susceptibility in the volume \( L^D \)

\[
\chi_2(T, L) = cL^D \exp (-fL^{2D}(T - T_c + dL^{-2D})^2) + \eta(T, L), \tag{24}
\]
with $c, d, e$ constants and $\eta(\cdot, L)$ analytic for $L < \infty$, locally uniformly convergent as $L \nearrow \infty$ (so that $\eta(\cdot, \infty)$ is analytic). With $v = L^{-D}, t = (T - T_c)/T_c$, it is straightforward to show that

$$\chi(t, v) := \chi_2(T, L)$$

belongs to $\Psi_1^\omega(U)$ for some $\omega$.

More generally, every function $\chi: U^* \to \mathbb{R}$ of the form

$$\chi(t, v) = \frac{1}{v} f(\frac{t}{v}) + \tilde{\chi}(t, v)$$

belongs to $\Psi_1^\omega(U)$ with appropriate $\omega > 0$, if the following conditions are satisfied.

1a. $\tilde{\chi}(t, v) \in C^1(U^*)$,

1b. $\tilde{\chi}(t, v)$ together with its (first) partial derivatives are uniformly bounded in $U^*$.

2a. $f \in C^1(\mathbb{R})$ is a nonnegative function with $f(0) > 0$,

2b. $\lim_{x \to \pm \infty} |x|^{1+\epsilon} f(x) = 0$ for some $\epsilon > 0$,

2c. $(d/dx) f(x)$ is uniformly bounded on $\mathbb{R}$.

Any such function has the property that it "approaches $\delta$" locally, i.e.

$$\lim_{\epsilon \to 0^+} \lim_{v \to 0^+} \int_{-\epsilon}^{\epsilon} dt \chi(t, v) > 0$$

and is finite. In this case the limits do not commute. An explicit example for such a function is

$$f(x) = \left(\frac{c}{\pi}\right)^{1/2} \exp(-cx^2), \ c > 0$$

with normalization

$$\int_{-\infty}^{\infty} dx f(x) = 1.$$ 

After these preliminaries we now state the following volume behaviour.

**Lemma 3.1** Let $\omega > 0$, $\chi \in \Psi_1^\omega(U)$. There are $\delta, \epsilon > 0$, and for every $t \neq 0$ there is $\nu_t > 0$ such that in $U^*$ for all $w, v, t$ with $v < \delta$ and $\nu_t w < |t| < \epsilon v$,

$$\chi(t, v) > |\chi(t, w)|.$$ 

In particular the lemma holds for $w = 0$, i.e.

$$\chi(t, v) > |\chi(t, 0)|.$$ 

This means that the susceptibility in that part of the transition region where $|t|/v < \epsilon$ is larger than in the infinite volume limit where $w = 0$. 


Proof: Let $\chi \in \Psi_1^\omega(U)$, $\omega > 0$. Differentiability implies that

$$\chi(t, v) = \chi(0, v) + t \int_0^1 ds \frac{\partial}{\partial \eta} \chi(\eta, v) \bigg|_{\eta=st}.$$

With appropriate $c_0, K > 0$ we have

$$\chi(0, v) \geq \frac{c_0}{v}$$

and

$$\left| \frac{\partial}{\partial \eta} \chi(\eta, v) \right| < \frac{K}{v^2}$$

in $U^\ast$. Hence

$$\chi(t, v) \geq \frac{c_0}{v} - \frac{|t|K}{v^2}.$$ 

Furthermore, for every $t \neq 0$ there is $\nu_t > 0$ such that

$$|\chi(t, w)| \leq \omega$$

for all $w < |t|/\nu_t$. Finally, we choose $\epsilon = c_0/(2K)$ and $\delta = c_0/(4\omega)$ and get for $v < \delta$ and $\nu_t w < |t| < \epsilon v$

$$\chi(t, v) \geq \frac{c_0}{v} - \frac{\epsilon K}{v^2} \geq \frac{c_0}{2v} > |\chi(t, w)|,$$

thus it follows the lemma. \hfill \Box

Now we come to the second order transition. In contrast to the first order case, at a second order transition the order parameter susceptibility can be divergent in the infinite volume limit as the critical temperature is approached. This is described by

**Definition 3.2** For any $\gamma > 0$ we denote by $\Psi_2^\gamma(U)$ the set of functions $\chi : U^\ast \to \mathbb{R}$ that are continuous and satisfy the following conditions.

1. There are constants $A$, $K$, $\epsilon > 0$ such that in $U^\ast$

$$|\chi(t, 0) - A |t|^{-\gamma}| \leq K |t|^{-\gamma+\epsilon}.$$

Furthermore, with appropriate $\nu$, $C > 0$, we have whenever $|t| > \nu v$,

$$\chi(t, v) \geq C \chi(t, 0).$$

2. There are constants $\eta$, $B > 0$ such that for $|t| < \eta v$

$$|\chi(t, v)| < B v^{-\gamma}.$$
The specific property for a 2nd order transition that the singular part of the free energy density behaves as a generalized homogeneous function implies for the susceptibility in a volume $L^D$ a typical form like

$$\chi_2(T, L) = |T - T_c|^{-\gamma} Q((T - T_c)L^{1/\nu}) + \eta(T, L),$$  \hspace{1cm} (26)

with some $\gamma > 0$. Here $\eta(\cdot, L)$ has similar analyticity properties as in (24) above, $\nu > 0$ is the critical exponent of the correlation length

$$\xi \sim |T - T_c|^{-\nu},$$ \hspace{1cm} (27)

$Q$ is continuous and behaves as

$$\lim_{x \to 0} |x|^{-\gamma} Q(x) = K > 0, \hspace{1cm} \lim_{x \to \pm\infty} Q(x) = C > 0.$$ \hspace{1cm} (28)

The first equation expresses the absence of a nonanalyticity of $\chi_2$ for finite $L$, the second one its presence in the infinite volume case. With $t = (T - T_c)/T_c$, $v = L^{-1/\nu}$ and

$$\chi(t, v) := \chi_2(T, L)$$

we see that $\chi$ belongs to $\Psi_2^\gamma(U)$ for some $\gamma$.

More generally, every function $\chi : U^* \to \mathbb{R}$ of the form

$$\chi(t, v) = \frac{1}{v^\gamma} f\left(\frac{t}{v}\right) + \bar{\chi}(t, v)$$ \hspace{1cm} (29)

with $\gamma > 0$ belongs to some $\Psi_2^\gamma(U)$, if the following conditions are satisfied.

1. $\bar{\chi}(t, v) \in C^1(U^*)$.
2a. $f \in C^1(\mathbb{R})$, and $f(0) > 0$,
2b. $\lim_{x \to \pm\infty} |x|^\gamma f(x) = C$ for some finite $C > 0$.

Compared to the first order case (24), the essential difference comes from property (2b).

As an example,

$$\chi(t, v) = (t^2 + v^2)^{-\gamma-\frac{m}{2}}, \hspace{0.5cm} m > 0,$$

belongs to the class $\Psi_2^m$.

For these functions, we have in contrast to Lemma (3.1)

**Lemma 3.2** Let $\gamma > 0$ and $\chi \in \Psi_2^\gamma(U)$. There are constants $\nu, \epsilon > 0, \nu < \epsilon$, such that for all $t, v, w$ with $\nu w < |t| < \epsilon v$

$$|\chi(t, v)| \leq \chi(t, w).$$
The inequality is always true if \( w = 0 \), i.e. the susceptibility is always smaller than in the infinite volume limit as long as we are in the critical region \( |t|/v < \epsilon \).

**Proof:** Let \( \chi \in \Psi_2^*(\mathcal{U}) \), \( \gamma > 0 \). There are numbers \( C, D, \nu > 0 \) such that in \( \mathcal{U}^* \) for \( |t| > \nu w \)

\[
\chi(t, w) > C \chi(t, 0) > D |t|^{-\gamma}.
\]

Furthermore, there are \( \eta, B > 0 \) such that for \( |t| < \eta v \)

\[
|\chi(t, v)| < B v^{-\gamma}.
\]

We choose \( \epsilon = \min (\eta, (D/B)^{1/\gamma}) \) and get for \( \nu w < |t| < \epsilon v \)

\[
|\chi(t, v)| < B v^{-\gamma} < B \left( \frac{\epsilon}{|t|} \right)^{-\gamma} < B \frac{\epsilon^\gamma}{D} \chi(t, w) < \chi(t, w).
\]

This proves the lemma. \( \square \)

Figure 1: \((t, v)\)-plane for susceptibilities \( \chi(t, v) > 0 \) in the vicinity of a phase transition at \((t = 0, v = 0)\), \( t \) denotes the scaling field \( t = (T - T_c)/T_c \), \( v \) is inverse to some power of the volume \( L^x \) with some \( x > 0 \). For a 1st order transition, \( \chi(t, v_1) > \chi(t, v_2) \), whereas for a 2nd order transition \( \chi(t, v_1) < \chi(t, v_2) \). For the shaded part no prediction is made.

\[
1/L^x \sim v \quad (t, v_1) \quad (t, v_2)
\]

### 3.2 The effective potential

Let us briefly discuss another method to determine the nature of a transition that will be of use later on. For definiteness we come back to the \( N \)-component scalar model as described in Section 2. A possible way to define an effective potential is by

\[
V \cdot V_{\text{eff}}(M) = - \Gamma(M)|_{M=\text{const}}, \quad (30)
\]

where \( V \) denotes the volume, and \( \Gamma(M) \) is defined by (11). In the symmetric phase and in the infinite volume limit, \( V_{\text{eff}} \) has to be convex. In practice, the right hand side of (30) is obtained as an expansion about \( M = 0 \). In the linked cluster expansion the coefficients can be expressed in terms of 1PI susceptibilities \( \chi_{n}^{1\text{PI}} \). They are obtained
as series representation in $\kappa$ of the truncated susceptibilities by keeping only those graphs that are 1PI [9]. Up to a constant we obtain

$$V_{\text{eff}}(M) = \frac{1}{2} \frac{1 - 4D\kappa\chi_{2}^{1\text{PI}}}{\chi_{2}^{1\text{PI}}} M^2 - \frac{1}{4!} \frac{\chi_{4}^{1\text{PI}}}{(\chi_{2}^{1\text{PI}})^4} (M^2)^2$$

$$- \frac{1}{6!} \frac{1}{(\chi_{2}^{1\text{PI}})^6} \left(\chi_{6}^{1\text{PI}} - \frac{10(\chi_{4}^{1\text{PI}})^2}{\chi_{2}^{1\text{PI}}^2}\right) (M^2)^3 + O(M^8).$$

Any nonconvex shape of $V_{\text{eff}}$ in the infinite volume limit must be an artifact of the approximation scheme. In a finite volume, however, a nonconvex shape in the symmetric phase signals a first order transition, whereas a convex shape is compatible with a second order transition. An estimate of the critical coupling is then obtained by a root of the coefficient of $M^2$ in the 2nd order case, and by degenerate values of $V_{\text{eff}}$ at the trivial and nontrivial minima in the 1st order case. In our applications (see Section 4) we have calculated the 1PI-susceptibilities $\chi_{2n}^{1\text{PI}}$ up to 16th order in $\kappa$ in a finite volume for $n = 1, 2, 3$.

4 Applications to scalar O(N) models with $\Phi^4$ and $\Phi^6$-point couplings

In this section we apply the methods discussed in the previous sections to the three-dimensional O(N) symmetric scalar model with $N = 1$ and $N = 4$. The model is described on a lattice $\Lambda$ by the partition function

$$Z(\kappa, \lambda, \sigma) = \int \prod_{x \in \Lambda} d^N \Phi(x) \exp (2\kappa \sum_{x,y \text{NN}} \Phi(x) \cdot \Phi(y) - \sum_{x} \hat{S} (\Phi(x), \lambda, \sigma)), \quad (32)$$

where the first sum of the exponential runs over unordered pairs of nearest neighbour lattice sites, and the ultralocal part $\hat{S}$ is given by

$$\hat{S} (\Phi, \lambda, \sigma) = \Phi^2 + \lambda(\Phi^2 - 1)^2 + \sigma(\Phi^2 - 1)^3 \quad (33)$$

with $\sigma > 0$ or $\sigma = 0$ and $\lambda \geq 0$. In contrast to the pure quartic interaction which only admits 2nd order transitions, the action (33) allows a richer phase structure with regions of 1st and 2nd order transitions due to the additional $\Phi^6$ interaction. The case of $\lambda = 3\sigma$ corresponds to a pure $\Phi^6$-theory, whereas $\lambda < 3\sigma$ implies a negative quartic coupling.

4.1 Preliminaries

To get a first estimate of the phase structure we consider the case of large couplings $\lambda$ and $\sigma$. For finite coupling constants we invoke a hopping mean field analysis.
The large coupling limit. To study the limit of large couplings, we set \( \lambda = \alpha \sigma \) and send \( \sigma \) to infinity with \( \alpha \) and \( \kappa \) kept finite and fixed. This limit is discussed for more general contact terms in Appendix A. The discussion is based on a saddle point integration. As a result we obtain the following behaviour in dependence on \( \alpha \). For \( \alpha > 1 \) and \( \alpha < -3 \) we obtain O(N) Heisenberg models (Ising model for \( N = 1 \)). The range of \(-3 < \alpha < 1\) leads to complete disordering with no phase transition at any finite \( \kappa \). The cases of \( \alpha = -1 \) and \( \alpha = 3 \) are peculiar. The resulting actions describe "diluted" O(N) models, with particular values of the couplings. If the large coupling limit is performed term by term in the HPE series it can be shown that at least for \( N \geq 2 \) the resulting actions again belong to the universality class of O(N) Heisenberg models.

A hopping-mean-field analysis. To get a first estimate of the phase structure at finite couplings, it is instructive to start with a mean field analysis. Together with the convexity of the exponential and the positivity of the measure this ansatz leads to a complete factorization of the partition function. The hopping mean field estimate for the free energy is then derived as follows. Let us define \( \hat{x} \) by

\[
\exp \hat{x}(H) = \int d^N \Phi \exp \left( - \sum_x \hat{S}(\Phi, \lambda, \sigma) + H \cdot \Phi \right),
\]

and the expectation value \( < F >_H \) of an observable \( F \) according to

\[
<F(\Phi)>_H = \exp (-|\Lambda| \hat{x}(H)) \cdot \int \prod_{x \in \Lambda} \left( d^N \Phi(x) \exp \left( - \sum_x \hat{S}(\Phi) + H \cdot \Phi \right) \right) F(\Phi).
\]

Here \( |\Lambda| \) denotes the lattice volume, and \( H \in \mathbb{R}^N \) is an auxiliary field. Note that \( \hat{x} \) defined in this way agrees with \( \hat{W} \) as introduced in Sect. 2. In particular, for every integer \( n \),

\[
\hat{v}_{2n}^c (\lambda, \sigma) = \left. \frac{\partial^{2n}}{\partial H_1^{2n}} \hat{x}(H) \right|_{H=0}
\]

(cp. to (11)). For simplicity, where no confusion can arise, we only indicate the dependence on \( H \). We get

\[
Z(\kappa, \lambda, \sigma) = < \exp (2\kappa \sum_{x,y \text{NN}} \Phi(x) \cdot \Phi(y)) >_H
\]

\[
\geq \exp < 2\kappa \sum_{x,y \text{NN}} \Phi(x) \cdot \Phi(y) >_H
\]

\[
= \exp (-|\Lambda| \overline{f}(H))
\]

with

\[
\overline{f}(H) = - \left( \hat{x}(H) + 6\kappa (\nabla H \hat{x}(H))^2 - H \cdot \nabla H \hat{x}(H) \right).
\]
An upper bound on the true free energy density $f$ is thus given by

$$f \leq \inf_H \overline{f}(H). \quad (34)$$

A vanishing $H_0 = 0$ is always a solution of the corresponding mean field equation

$$\partial_H \overline{f}(H_0) = -\partial^2_H \hat{x}(H_0) \left( 12 \kappa \partial_H \hat{x}(H_0) - H_0 \right) = 0,$$

where the derivative is in the direction of $H$, and $H_0 = 0$ is a local minimum of $\overline{f}$, if

$$\partial^2_H \overline{f} = \partial^2_H \hat{x}(H_0) \left( 1 - 12 \kappa \partial^2_H \hat{x}(0) \right) > 0. \quad (35)$$

In particular, for small hopping parameter $\kappa$ the model is always in the symmetric phase.

This form of mean field analysis is identical to the tree level of the hopping parameter expansion. It can be easily shown that the Lebowitz inequality

$$\partial^3_H \hat{x}(H) < 0 \quad \text{for all } H > 0$$

together with $\partial^2_H \hat{x}(H) > 0$ for all $H$ ensures that $H_0 = 0$ is the absolute minimum of $\overline{f}$. The Lebowitz inequality holds in any case for $\lambda \geq 3\sigma$. Equality in (35) along with

$$\partial^4_H \overline{f}(0) > 0 \quad (36)$$

locates a 2nd order phase transition to the spontaneously broken phase at

$$\kappa_c(\lambda, \sigma) = \frac{1}{12 \hat{v}^c_2(\lambda, \sigma)}.$$

Tricritical points are identified by an equality in (35) and

$$\partial^6_H \overline{f}(0) > 0,$$

i.e.

$$\hat{v}^c_4(\lambda, \sigma) = 0 \quad \text{and} \quad \hat{v}^c_6(\lambda, \sigma) = 0.$$

We notice that these conditions imply a vanishing two and four-point coupling in the effective potential $V_{\text{eff}}$, Eq.(31), evaluated to tree level in the HPE, i.e. in the hopping mean field approximation. Thus the criterion for tricriticality reduces to the familiar one. If we had used the classical potential (33) instead, this would lead to a location of the tricritical line in the bare coupling constant space at $\lambda = 3\sigma$.

In Table 1 we have listed some results for the O(4)-model on the location of the tricritical line in the $(\lambda, \sigma)$-space for several values of $\alpha$.

The tricritical exponents in hopping-mean-field establish the results of the most naive mean field analysis with the effective potential replaced by the classical potential. They are $\alpha = 1/2, \beta = 1/4, \gamma = 1, \delta = 5, \nu = 1/2$. From the Ginzburg criterion one may expect that the only chance where a mean field type of analysis may lead to reliable predictions of the singular behaviour in three dimensions is at tricriticality. In fact, the susceptibility comes out as volume independent along the tricritical line (cf. Section 4.3 below) when it is determined by the HPE analysis. A mean field analysis is volume independent by construction.
Table 1: Mean field tricritical line for the O(4) model on the three-dimensional hypercubic lattice. The line is defined by $v_4^c = 0$ and $v_6^c < 0$, $\sigma$ is defined by $\sigma = v_6^c / (5v_2^c)^3$.

| $\alpha$ | $\lambda = \alpha \sigma$ | $\sigma$ | $\tilde{\sigma}$ |
|----------|-----------------|--------|----------------|
| 1/1.05   | 128.199         | 134.609| -0.7245305     |
| 1/1.1    | 53.040          | 58.344 | -0.6875585     |
| 1/1.2    | 21.822          | 26.286 | -0.5920738     |
| 1/1.3    | 13.252          | 17.228 | -0.5193738     |
| 1/1.5    | 7.315           | 10.973 | -0.4451270     |
| 1/2.0    | 3.401           | 6.802  | -0.3839411     |
| 1/5.0    | 0.788           | 3.941  | -0.3407590     |
| 1/10.0   | 0.344           | 3.494  | -0.3345469     |
| 1/100.0  | 0.031           | 3.081  | -0.3306763     |
| -1/10.0  | -0.273          | 2.731  | -0.3284753     |
| -1/1.1   | -1.391          | 1.530  | -0.3519023     |
| -1.0     | -1.472          | 1.472  | -0.3581768     |
| -2.0     | -2.948          | 1.474  | -0.5106579     |
| -3/1.2   | -7.561          | 3.024  | -0.6827047     |
| -3/1.1   | -17.678         | 6.482  | -0.7259408     |

4.2 Infinite volume analysis at finite couplings

So far we have studied the phase structure in the large coupling limit and in a mean field analysis for finite couplings. Next we utilize the linked cluster expansions for a more thorough study. Susceptibilities are represented as convergent power series in the hopping parameter, such as the $2n$-point functions

$$\chi_{2n}(\kappa, \lambda, \sigma) = \sum_{\mu \geq 0} a_{\mu}^{(2n)}(\lambda, \sigma) \kappa^\mu,$$

(38)

and similarly for weighted correlations. These series have been computed to 20th order in $\kappa$ for $n = 1$, to 18th order for $n = 2$, and to 16th order for $n = 3$, both in a finite and infinite volume. In the infinite volume, the coefficients of the series we have explicitly calculated are of equal sign for each series. Under the assumption that this behaviour continues to all orders in $\kappa$, the radius of convergence $\kappa_c(\lambda, \sigma)$ is identified with the singularity closest to the origin on the positive real axis, hence with the physical singularity at the phase transition, independently of the order of the transition.

Well developed methods are known to obtain critical data from the high order coefficients of high temperature series [4, 19]. The critical point $\kappa_c(\lambda, \sigma)$ is identified by the ratio criterion, applied to the coefficients $a_{\mu}^{(2n)}(\lambda, \sigma)$. The best choice is the
2-point susceptibility, because its series is available to the highest order. The obliged regression towards large \( \mu \) is done according to

\[
r_\mu := \frac{a^{(2)}_\mu}{a^{(2)}_{\mu-1}} = \frac{1}{\kappa_c} \left( 1 + \frac{c_1}{\mu^{\omega_1}} + O(\mu^{-\omega_2}) \right)
\]

(39)

with \( \omega_2 > \omega_1 > 0 \), \( c_1 \) as fit parameter chosen according to the best \( \chi^2/df \) fit. This procedure is eventually supplemented by a shift of the weak antiferromagnetic singularity at \( -\kappa_c \) to \( -\infty \), an improved estimator fit and other known techniques like Padé methods. We know that \( \omega_1 = 1 \) for a leading pole or branch point singularity on the real axis, i.e. for

\[
\chi_2 \simeq A (\kappa_c - \kappa)^{-\gamma} \quad \text{as } \kappa \nearrow \kappa_c
\]

with \( \gamma > 0 \) and \( \gamma \neq 1 \), and \( \omega_1 > 1 \) for \( \gamma = 1 \). For a 2nd order transition, an alternative way to determine the critical point is given by the smallest real solution of

\[
12 \kappa_c \chi_2^{1\text{PT}}(\kappa_c) = 1,
\]

as proposed in \[9\]. This condition is equivalent to the identification of the phase transition as a zero of the quadratic coefficient of the effective potential, cf. \[21\]. It turns out to be the most convenient way to determine the radius of convergence leading to the highest precision in \( \kappa_c \). The lowest precision obtained in this way lies within 4-5 digits. Once \( \kappa_c \) is determined we obtain the critical exponent \( \gamma \) from

\[
1 + \mu(\kappa_c r_\mu - 1) = \gamma + \frac{c_2}{\mu^{\omega_3}} + o(\mu^{-\omega_3}),
\]

(40)

with \( \omega_3 \) and \( c_2 \) as fit parameters. In a similar way, the critical exponent \( \nu \) is obtained by replacing the series of \( \chi_2 \) by that of \( m_R^{-2} \), cf. \[8\].

A measurement of critical exponents like \( \gamma, \nu, \eta \) leads to a qualitative plot of the phase structure in the \((\lambda, \sigma)\)-halfplane as shown in Fig. 4. The solid line represents the boundary \( \lambda = \lambda_\sigma(\sigma) \) between the 2nd and 1st order region. To the left of this tricritical line the phase transition is of 2nd order. Here, except for the origin \( \lambda = \sigma = 0 \), we obtain one universality class for every \( N \) with plateaus of critical exponents, with values of the \( N \)-component Heisenberg model (cf. e.g. \[1\] for a recent list of those exponents). It is remarkable that this range considerably extends the "Lebowitz domain" \( \lambda \geq 3\sigma \), where the action is convex and therefore \( \gamma \) is not less than 1 \[20\]. In particular, it includes the full range of \( \lambda < -3\sigma \). In passing we mention that for \( \lambda \geq 0 \) the presence of a small nonvanishing \( \Phi^6 \) interaction, that is \( \sigma > 0 \), considerably accelerates the convergence of the high temperature series compared to the case \( \sigma = 0 \), i.e. the non-universal remainder of \([8]\) becomes smaller.

Except for the values of the critical exponents, the phase structure qualitatively confirms the mean field analysis of the last subsection. As the tricritical line \( \lambda = \)}
Figure 2: Qualitative plot of the phase structure of $O(N)$ lattice models in 3 dimensions. The dashed curves give the lines $\lambda = \alpha \sigma$ with $\alpha = 1$ and $\alpha = -3$. The solid curve represents the tricritical line $\lambda_t(\sigma)$. To the left of it the phase transition is of 2nd order, to the right of it 1st order.

$\lambda_t(\sigma)$ is approached, the exponents $\gamma$ and $\nu$ drop continuously from their values in the Heisenberg models to the Gaussian values, where the tricritical line is crossed, and further to zero. The smooth interpolation between the different exponents is an artifact of the truncation of the power series expansions at high, but finite order in $\kappa$. It was already pointed out in [9] that various universality classes lead to smearing effects at finite order due to an “interference” of various universality domains. The most pronounced plateau structure is obtained for $\nu \eta$, the critical exponent of the wave function renormalization constant $Z_R$. In Fig. 3 we show the results on the exponent $\nu \eta$ for the $O(4)$ model, obtained from the 20th order susceptibility series of $\chi_2$ and $\mu_2$, (5), for various $\sigma$ along the ray $\lambda = (1/2)\sigma$. There is a well established plateau at the left part of the plot corresponding to the universality class of the Heisenberg model. The plateau at the right part is compatible with a range of 1st order transitions, all exponents $\gamma, \nu, \eta$ vanish within the error bars. Hence they are compatible with a finite correlation length at $\kappa_c$. The stability of the extrapolated convergence radius $\kappa_c$ under a variation of the truncation of the series suggests that there is really a 1st order transition rather than a mere crossover phenomenon. We would like to identify the left boundary of this plateau as the tricritical point. This gives us an estimate of about $\sigma_t \approx 9.0$. The indicated errors in Fig. 3 are obtained as discussed in connection with (40). The smearing effect does not allow for a more precise location of the tricritical point. To
get a clearer identification of the 1st order transition region and a better localization of the tricritical point it is natural to perform a finite size scaling analysis, which is the topic of the next section.

4.3 Results of the finite size scaling analysis

In Sect. 3 we have formulated monotony criteria for response functions $\chi$ in the scaling region. In absolute value, increase in volume implies a 2nd order transition, decrease in volume a 1st order one. The response functions have to be calculated at some $\bar{\kappa}$ close to but not at the critical point $\kappa_c$ for two volumes. The value of $\bar{\kappa}$ should be chosen sufficiently close to the transition point to satisfy the conditions of the monotony criterion, and sufficiently apart from $\kappa_c$ to allow a use of the truncated series representation. A choice of $\bar{\kappa} = 0.98\kappa_c(\lambda, \sigma)$ fulfills both restrictions.

The volumes should be sufficiently large in lattice units to guarantee the applicability of the finite size scaling ansatz for $\chi$. Beyond this generic condition the following restrictions arise from the monotony criterion. The smaller one of the two volumes should satisfy $L^x|\bar{\kappa} - \kappa_c| \lesssim 1$ with $x = 1/\nu$ or $x = 3$, which implies an upper bound on $L$ for given $\bar{\kappa}$. In practice we have chosen this $L$ between 4 and 12.
In the context of the HPE the larger one of the two volumes may be set to infinity. The advantage of this choice is that in the 1st order case, decrease in volume holds all over the scaling region. In Monte Carlo simulations the second volume is necessarily finite. In this case \( L \) should be large enough so that \( \tilde{\kappa} \) lies outside the small neighbourhood of \( \kappa_c \) where \( \chi \) is increasing in the 1st order case as well. The critical point \( \kappa_c(\lambda, \sigma) \), which enters the inequalities on \( L \) and \( \tilde{\kappa} \), is determined as the radius of convergence in the infinite volume as described above.

We use the 2-point susceptibility, because its series is available to the highest order in \( \kappa \). For given couplings \( \lambda \) and \( \sigma \)

\[
\chi_2^{(M)}(\tilde{\kappa}, \lambda, \sigma; L) = \sum_{\mu=0}^{M} a^{(2)}_{\mu}(\lambda, \sigma; L) \tilde{\kappa}^\mu
\]  

(41)
denotes the 2-point susceptibility truncated at order \( M \). With

\[
r_M(\lambda, \sigma; L) := 1 - \frac{\chi_2^{(M)}(\tilde{\kappa}, \lambda, \sigma; L)}{\chi_2^{(M)}(\tilde{\kappa}, \lambda, \sigma; \infty)},
\]  

(42)
we know that \( r_\infty(\cdot; L) > 0 \) for 2nd order and \( r_\infty(\cdot; L) < 0 \) for 1st order transitions, if \( L \) lies within the bounds as explained above. The convergence of the series (41) as \( M \to \infty \) ensures the same behaviour for finite, but sufficiently large \( M \).

Fig. 4 shows an application of the monotony criteria to the 1-component model. We have plotted the volume dependence of the ratios \( r_M(\lambda, \sigma; L) \) for a truncation at order \( M = 20 \) and for various lattice sizes \( L = (L_1 L_2 L_3)^{1/3} \), at two points of the bare coupling constant space. One point is well inside the 1st order region, the other one well inside the 2nd order part of the phase diagram, the different areas have been identified by the infinite volume series as discussed in the last subsection. Clearly the sign of \( r_{20}(\cdot; L) \) is different in both regions of phase space. It is positive for the 2nd order transition and negative for the 1st order transition. The approach to the infinite volume limit where \( r_M(\cdot; \infty) = 0 \) is fast.

Next we want to demonstrate how one can utilize the finite volume criteria with HPE to get a better localization of the tricritical region. Let us consider the O(4) model and determine the behaviour of the ratios \( r_M \) along the line \( \lambda = (1/2) \sigma \). From the infinite volume analysis of the last subsection we had obtained \( \sigma_t \simeq 9.0 \) as an estimate for the tricritical coupling \( \sigma_t \).

Since \( r_M(\lambda, \sigma; L) > 0 \) for 2nd order and < 0 for 1st order transitions, the tricritical point should be localized at the zero of \( r_M(\lambda, \sigma; L) \) between these two ranges (with nonvanishing slope, i.e. \( \partial r_M(\sigma/2, \sigma; L) / \partial \sigma \neq 0 \)), suitably extrapolated to \( M, L \to \infty \).

Fig. 5 shows the ratios \( r_M(\sigma/2, \sigma; L) \) as function of \( \sigma \) for \( L = 4 \) and various \( M \) between 0 (corresponding to the mean field approximation) and 20. The intersections of the curves with the \( r = 0 \)-axis lie in the range of \( 8 \leq \sigma \leq 8.5 \). The zeroes \( \sigma_M(L) \), defined by \( r_M(\sigma_M(L)/2, \sigma_M(L); L) = 0 \), depend on the order \( M \) at which
the susceptibility series of $\chi_2$ have been truncated and on the lattice size $L$. The dependence on $L$ for fixed $M$ of $r_M(\lambda, \sigma; L)$ is shown in Fig. 3.

Thus a final localization of the tricritical coupling $\sigma_t$ needs an extrapolation in $L$ and $M$ to infinity. Clearly both extrapolations are not independent of each other. We should expect that a comparison of two ratios is sensible, i.e.

$$r_M(\cdot; L) \simeq r_{M'}(\cdot; L')$$

if lattice sizes $L, L'$ and truncation $M, M'$ satisfy

$$\frac{M}{L} = \frac{M'}{L'}.$$  \hfill (44)

The reason is that $M/L$ is the maximal number of times a graph contributing to the series of $\chi_2(M)(\cdot; L)$ can wind around the volume. Eq. (44) then ensures that the remaining $L$-dependence becomes independent of $M$ for sufficiently large $M$.

Fig. 7 shows the data $\sigma_M(L)$ obtained on a $4^3$-lattice ($L = 4$), and for $11 \leq M \leq 20$, as a function of $1/M$. The curves show the regression

$$\sigma_M(4) = \sigma_t(M_{\text{min}}, L = 4) + \frac{\delta(M_{\text{min}})}{M}. $$
Figure 5: The ratios $r_M(\lambda, \sigma; L)$ as function of $\sigma$ for $\lambda = \sigma/2$, and $L = 4$, i.e. on a $4 \times 4 \times 4$-lattice.

as obtained for $M_{\text{min}} \leq M \leq 20$, and for $M_{\text{min}} = 14, 16, 18$. In Fig. 8 we show the second regression for the resulting $\sigma_t(M_{\text{min}}L/4, L)$ in $1/M_{\text{min}}$, for $L = 4, 6$

$$\sigma_t(M_{\text{min}}L/4, L) = \sigma_t + \frac{\epsilon}{M_{\text{min}}},$$

leading to the final prediction of $\sigma_t$. We have scaled the adjusted $M_{\text{min}}$ according to (44). Note that both data sets, on the $4^3$ and on the $6^3$-lattice, fall on the same straight line within the error bars. We obtain

$$\sigma_t = 9.454(49).$$

In passing we remark that the accuracy of $\sigma_t$ has been increased by at least one order of magnitude compared to the infinite volume analysis (Fig. 3). It should be noticed that the volume independence of $\chi_2$ in the scaling region of the tricritical point just confirms the validity of a mean field analysis of tricritical exponents. A mean field analysis is volume independent by construction. The expected volume independence of $\chi_2$ is confirmed within the error bars.

In the remainder of this section we discuss the volume dependence of the radius of convergence and of the effective potential.

*Shift and scaling of $\kappa_c(\lambda, \sigma; L)$.* We define $\kappa_c(\lambda, \sigma; L)$ in the finite and infinite volume as the radius of convergence of the susceptibility series, in particular of $\chi_2$,
which is known including the 20th order. Some data for $\kappa_c(L)$ are listed in Table 2 for a three-dimensional O(1) and O(4) model. The couplings $(\lambda, \sigma)$ for each $N$ ($N = 1, 4$) have been chosen deeply in the 1st order transition region.

From a finite size scaling analysis one expects (cf. Sect. 3) that the data should fit with a regression in $L$ according to

$$|\kappa_c(\cdot; L) - \kappa_c(\cdot; \infty)| \simeq \ln c - y_T \ln L$$

for large $L$, with some constant $c$ and a critical exponent $y_T$. For the $\mathbb{Z}_2$ model we obtain in the 1st order transition region ($\lambda = 15/1.1, \sigma = 15.0$) according to Table 2

$$\ln c = 4.57(57)$$
$$y_T = 6.21(32)$$

with $\chi^2/df = 0.025$. Thus the scaling behaviour is consistent with $y_T = 2D = 6$. It confirms the behaviour which has been predicted for the shift of the critical coupling determined as the maximum of the susceptibility in a class of models which cover the $\mathbb{Z}_2$ model [18]. Note that it is in disagreement with the Gaussian two-peak model [16], predicting a leading finite size correction proportional to $L^{-D}$, which one might have expected.

The same scaling behaviour is found for the O(4) model in the 1st order transition
Figure 7: The solution $\sigma_M(L)$ of the equation $r_M(\sigma_M(L)/2, \sigma_M(L); L) = 0$ for $L = 4$, plotted against $1/M$, $M$ is the order of truncation of the susceptibility series. Regression is shown as a linear function of $1/M$ for $M \geq M_{\text{min}}$ with $M_{\text{min}} = 14, 16, 18$.

region. Here we get (Table 2)

\begin{align*}
\ln c &= 4.57(120) \\
y_T &= 5.55(59).
\end{align*}

Thus a leading correction proportional to $L^{-3}$ lies clearly outside the error bars. This result is remarkable, because the $O(4)$-model (which is a Heisenberg model in the large coupling limit) is not covered by the analysis of Borgs, Imbrie, Kotecky and Miracle-Sole [17, 18]. Hence the vanishing of the coefficient of the linear term in a large volume expansion of the susceptibilities in powers of $1/L^3$ seems to be a universal feature of a large class of models.

A measurement of the scaling behaviour of $\kappa_c(L)$ in the 2nd order region of the $O(4)$ model was not conclusive, because the shift of $\kappa_c$ occurs in the 4th or 5th digits, hence the finite size effect is hidden in the error. In the 2nd order region of the $\mathbb{Z}_2$ model we measure a scaling, which is best fitted by an ansatz (cf. Table 3)

$$\kappa_c(\cdot; L) = \kappa_c(\cdot; \infty) + \frac{c}{L^{y_T}}$$

with $y_T = 2/\nu$, and

$$\ln c = -2.25(129)$$
Figure 8: The "scaled" solutions $\sigma_t(M_{min}L/4, L)$, plotted against $1/M_{min}$, for $L = 4$ and $L = 6$. Within the error bars, the data are on a straight line, thus confirming the assumptions made in connection with Eqns. (43) and (44). Linear regression in $1/M_{min}$ gives the tricritical point.

$$y_T = 2.83(59)$$

with $\chi^2/df = 0.1$. From a renormalization group analysis one expects a leading scaling correction proportional to $L^{-1/\nu}$. Also here the finite size effect is not large compared to the error in $\kappa_c$, thus the disagreement with an $L^{-1/\nu}$-behaviour may be due to the errors in $\kappa_c$ and the uncertainty in the involved extrapolations.

We conclude the discussion of $\kappa_c(L)$ with a conjecture concerning the monotony behaviour.

Monotony in $\kappa_c(L)$. The results of Table 3 for $\kappa_c(L)$ exhibit a further characteristic distinction between 1st and 2nd order transitions. Since we are not aware of a general proof, we leave it as a

Conjecture: The convergence radius $\kappa_c(L)$ of the series expansions is monotonically decreasing with $L$ for 2nd order transitions, and monotonically increasing for 1st order transitions.

The effective potential as function of $L$. Similarly we have measured $V_{eff}$, Eq. (31), for two points well inside the supposed 1st and 2nd order transition regions of the O(4) model ($\lambda = 6.0$, $\sigma = 12.0$, and $\lambda = 0.90$, $\sigma = 1.0$, respectively). The
Table 2: Radius of convergence $\kappa_c(L)$ of the HPE series for the 1st order region. It is determined from the 2-point susceptibility series, as described in Section 4.2. Data are given for the 3d $\mathbb{Z}_2$ and O(4) model, for various volumes $L^3$.

| $L$ | $\mathbb{Z}_2$ | $O(4)$ |
|-----|----------------|--------|
| $\infty$ | 0.51047(1) | 0.84462(10) |
| 4 | 0.49381 | 0.79531 |
| 6 | 0.50886 | 0.83851 |
| 8 | 0.51025 | 0.84416 |
| 10 | 0.51047 | 0.84436 |
| 12 | 0.51047 | 0.84447 |

Table 3: Radius of convergence $\kappa_c(L)$ of the HPE series for the 2nd order region in the $\mathbb{Z}_2$ model for various volumes $L^3$.

| $L$ | $\lambda = 3.0$, $\sigma = 1.0$ |
|-----|----------------|
| $\infty$ | 0.17316(4) |
| 6 | 0.17393 |
| 8 | 0.17339 |
| 10 | 0.17327 |
| 12 | 0.17327 |

$\chi_{1PI}^{1PI}$ entering Eq. (31) have been evaluated to 16th order in $\kappa$ for $n = 1, 2, 3$ in a finite and infinite volume. For the 2nd order point $\lambda = 0.90$, $\sigma = 1.0$, and for volumes $L^3$ with $L = 4, 6$ and infinity, $V_{eff}$ is convex in the symmetric phase up to a resolution of $10^{-8}$.

In the first order case (Fig. 9) $V_{eff}$ is nonconvex in the symmetric phase with a barrier height decreasing with increasing $L$. The three curves correspond to a $4^3$, $6^3$ and $\infty^3$ lattice, respectively. Note that the nonconvex shape which is even seen for the $\infty^3$ lattice (lowest barrier in Fig. 9) must be attributed to the approximation scheme, i.e. to the truncation at order $M = 16$. (As mentioned above, the truncation of the series expansion acts similarly to a finite volume cut-off. The finite volume leads to a nonconvex shape only in the 1st order case. Thus it is not surprising that we find a convex shape in the symmetric phase for all volumes in the 2nd order case, in spite of the same truncation in $M$.)
Figure 9: Volume dependence of the effective potential $V_{\text{eff}}(\Phi)$ on lattices with varying size $L^3$. The barrier height decreases with $L$. The curves are obtained for $L = 4, 6, \infty$. The parameters are $\lambda = 6.0, \sigma = 12.0$ in the 3d O(4)-model.

The coexistence of minima leading to the same value of $V_{\text{eff}}$ defines a critical coupling $\tilde{\kappa}_c(L)$ which need not agree with the finite volume convergence radius $\kappa_c(L)$, unless the truncated expansions of $V_{\text{eff}}(\Phi)$ in $\Phi$ and of $\chi_2^{PI}$ in $\kappa$ are extrapolated to infinity. For parameters chosen as in Fig. 9 we find $\tilde{\kappa}_c(4) = 0.8311$, $\tilde{\kappa}_c(6) = 0.8475$, $\tilde{\kappa}_c(\infty) = 0.8488$, in contrast to $\kappa_c(4) = 0.7953$, $\kappa_c(6) = 0.83851$, $\kappa_c(\infty) = 0.84462$, cf. Table 2, determined as the radius of convergence of the series expansions, extrapolated to infinite $M$.

*Tricritical parameters from $V_{\text{eff}}$.* Vanishing coefficients of the $\Phi^2$ and $\Phi^4$-terms associated with a qualitative change in the shape of $V_{\text{eff}}$ provide a further possibility for localizing the tricritical couplings. The analytical dependence of the coefficients on $\lambda$ and $\sigma$ is rather indirect. It is easier to determine $\lambda_t$, $\sigma_t$ by the first occurrence of a nonconvex shape of $V_{\text{eff}}$ in the symmetric phase, coming from the 2nd order transition region. The highest order, which is so far available for the six-point susceptibility $\chi_6^{PI}$, entering the $\Phi^6$-coefficient of $V_{\text{eff}}$, is 16. The number of contributing graphs to order 16 is comparable to the number of graphs contributing to the two-point susceptibility to order 20 and the four-point susceptibility to order 18. An inclusion of higher powers in $\Phi$, say $\Phi^8, \Phi^{10}$-terms, would further reduce the order in $\kappa$ which is tractable. Thus we retain from further extrapolations, but give
bounds on $\sigma_t$, derived from $V_{eff}(\Phi)$ to $O(\kappa^{16})$. They are

$$9.75 \leq \sigma_t \leq 10.0.$$  \hspace{1cm} (46)

The resolution in $V_{eff}$, within which no nonconvex shape was seen up to $\sigma = 9.75$, was $10^{-7}$. Compared to the more reliable result of Eq. (45), the evaluation of $V_{eff}$ seems to lead to an upper bound on $\sigma_t$, given by Eq. (46).

5 Summary and Outlook

In this paper we have generalized hopping parameter expansions from an infinite to a finite volume. The combination of performing the expansions in a finite volume and to a high (20th) order in the expansion parameter has turned out as a useful computational technique to approach the critical region from the symmetric phase and, in addition, to characterize the type of transition. First and second order transitions have been distinguished by various criteria: the monotony criterion referring to the $L$-dependence of response functions (here illustrated at order parameter susceptibilities), the scaling and monotony of the radius of convergence $\kappa_c(L)$ as function of the linear lattice size $L$, and the effective potential as function of $L$. In particular, it is the different $L$-dependence of the order parameter susceptibility for 1st and 2nd order transitions in the scaling region (close to but not at the transition point) which allows us to localize tricritical points. The monotony criterion can be applied to Monte Carlo simulations as well, the involved two volumes should be sufficiently large, but both may be finite.

We have applied these methods to renormalizable $O(N)$ models in three dimensions. The plateau structure in the critical exponent $\nu_\eta$ in the infinite volume has revealed two universality classes belonging to an $O(N)$-Heisenberg model and to a Gaussian model. Apart from the ”trivial” Gaussian behaviour at vanishing four and sixpoint couplings, we get Gaussian exponents along a tricritical line separating 1st and 2nd order domains. The existence of the 1st order domain and the tricritical line is based on the presence of the $\Phi^6$ self-interaction. The $O(N)$ symmetry alone does not determine the critical behaviour.

Several extensions are at hand. The first one is from 3 dimensions to field theories in four dimensions at finite temperature. For a $\Phi^4 + \Phi^6$-type theory in four dimensions at finite temperature we expect qualitatively the same infrared behaviour and phase structure as for three dimensions, but different values for the critical couplings. A check of the supposed dimensional reduction from four to three dimensions is of particular interest in connection with the electroweak phase transition. $\Phi^6$ terms in the dimensionally reduced $SU(2)$-Higgs model are usually argued to be irrelevant even at the transition to the spontaneously broken phase, and hence dropped [21]. In our extension of the previous investigations we will keep the $\Phi^6$ term in a 4d effective scalar theory at finite temperature, which is derived from the underlying $SU(2)$-Higgs model by integrating out the gauge field degrees
of freedom. The phase structure of the effective scalar theory will then be studied in a finite and infinite volume. Hopping parameter expansions are supposed to work the better the smaller $\kappa$, thus the larger the Higgs masses. Hence this investigation complements the range of Higgs masses which has been available in recent Monte Carlo simulations [22]. One of our aims is to find the critical Higgs mass above which the electroweak phase transition ceases to exist. (In case that the physical Higgs mass lies above the critical Higgs mass, it is bad news for an explanation of the observed baryon number asymmetry in the universe. The necessary ingredient for an out-of-equilibrium situation can no longer be provided by the electroweak transition, if the ”transition” turns out to be truly a smooth crossover phenomenon.)

A further application of our computational tools are (tri)critical phenomena in statistical physics. The order of the transition in a superconductor of type II has been recently under debate ([23] and references therein.) The existence of a tricritical point for a suitable Ginzburg-Landau parameter has been conjectured [24], but a proof of its existence is still outstanding. Work in both directions is in progress.

A Large coupling limit of O(N) lattice models

For $N \geq 1$, on a $D$-dimensional hypercubic lattice $\Lambda$, we consider the partition function

$$Z = \int D\Phi \exp (-S(\Phi))$$

with corresponding expectation values

$$< P >_{\lambda,\sigma} = \frac{1}{Z} \int D\Phi P(\Phi) \exp (-S(\Phi)),$$

where

$$D\Phi = \prod_{x \in \Lambda} d^N\Phi_x$$

and

$$S(\Phi) = -\frac{1}{2} \sum_{x \neq y} v_{xy} \Phi_x \cdot \Phi_y + \sum_x S^\circ (\Phi_x),$$

$$S^\circ (\Phi) = \Phi^2 + \lambda(\Phi^2 - 1)^2 + \sigma(\Phi^2 - 1)^3.$$
\[ \sum_{y \in \Lambda} v_{xy} < \infty, \quad (48) \]
\[ \sum_{x,y \in \Lambda} v_{xy}(\Phi_x - \Phi_y)^2 \geq 0. \]

As an example, these conditions are satisfied for the pure nearest neighbour interaction, where
\[ v_{xy} = 2\kappa \sum_{\mu=0}^{D-1} (\delta_{x,y+\hat{\mu}} + \delta_{x,y-\hat{\mu}}), \quad (49) \]
with \( \hat{\mu} \) denoting the unit vector in \( \mu \)-direction. We consider (47) in the limit \( \sigma \to \infty \) with \( \lambda = \alpha \sigma \) and \( \alpha \) a fixed real number, i.e.
\[ \langle P \rangle_\alpha = \lim_{\sigma \to \infty} \langle P \rangle_{\alpha \sigma \sigma} \]
for
\[ \tilde{S}(\Phi) = \Phi^2 + \sigma(\Phi^2 - 1)^2(\Phi^2 - 1 + \alpha). \]

The hopping parameters \( v_{xy} \) are considered as fixed. We have to select all field configurations that minimize the action in this limit. It is convenient to parametrize the fields according to
\[ \Phi_x = u_x v_x, \quad u_x \in S_{N-1} \text{ (the N-1 sphere)}, \quad v_x \geq 0. \]

**Lemma A.1** As \( \sigma \to \infty \) we get the following behaviour of expectation values \( P \) in dependence on \( \alpha \)

\( \alpha > 1 \):
\[ \langle P \rangle_\alpha = N_\alpha \prod_{x \in \Lambda} \left( \int_{S_{N-1}} d\Omega_{N-1}(u_x) \right) P(u) \exp(-\tilde{S}(u)), \]
\[ \tilde{S}(u) = -\frac{1}{2} \sum_{x,y \in \Lambda} v_{xy} u_x \cdot u_y. \]

\( \alpha = 1 \):
\[ \langle P \rangle_1 = N_1 \prod_{x \in \Lambda} \left( \sum_{v_x=0,1} \left( \int_{S_{N-1}} d\Omega_{N-1}(u_x) \delta_{v_x,1} + \delta_{v_x,0} \right) \right) P(uv) \exp(-\tilde{S}(u,v)), \]
\[ \tilde{S}(u,v) = \sum_{x \in \Lambda} v_x^2 - \frac{1}{2} \sum_{x,y \in \Lambda} v_{xy} v_x v_y u_x \cdot u_y. \]

\( -3 < \alpha < 1 \):
\[ \langle P \rangle_\alpha = P(0). \]
\( \alpha = -3: \)

\[
< P >_{-3} = \mathcal{N}_{-3} \prod_{x \in \Lambda} \left( \sum_{u_x = 0, 1} \left( \int_{S_{N-1}} d\Omega_{N-1}(u_x) \delta_{\nu_x, 1} + \delta_{\nu_x, 0} \right) \right) P(\sqrt{3uv}) \exp (-\tilde{S}(u, v)),
\]

\[
\tilde{S}(u, v) = \sum_{x \in \Lambda} 3v_x^2 - \frac{3}{2} \sum_{x, y \in \Lambda} v_xyv_yu_x \cdot u_y.
\]

\( \alpha < -3: \)

\[
< P >_{\alpha} = \mathcal{N}_{\alpha} \prod_{x \in \Lambda} \left( \int_{S_{N-1}} d\Omega_{N-1}(u_x) \right) P((1 - \frac{2\alpha}{3})u) \exp (-\tilde{S}(u)),
\]

\[
\tilde{S}(u) = -\frac{1}{2} \sum_{x, y \in \Lambda} (1 - \frac{2\alpha}{3})v_xyu_x \cdot u_y.
\]

The \( \mathcal{N}_{\alpha} \) are positive normalization factors independent of \( P \) such that \( 1 >_{\alpha} 1 \), \( d\Omega_{N-1} \) is the standard measure on the sphere.

For \( \alpha > 1 \) and \( \alpha < -3 \) we obtain the \( O(N) \) Heisenberg model (Ising model for \( N=1 \)). For \( -3 < \alpha < 1 \) the lattice model becomes completely decoupled. At the boundary points \( \alpha = 1 \) and \( \alpha = -3 \) the result are “diluted” \( O(N) \) models, i.e. \( O(N) \) models with additional occupation number variables \( v_x \in \{0, 1\} \).

Outline of the proof: The properties (48) ensure that the minimizing field configurations of the action \( S(\Phi) \) are translation invariant. Thus it is sufficient to determine the minima of

\[
F(\Phi) = (\Phi^2 - 1)^2(\Phi^2 - 1 + \alpha), \quad \Phi \in \mathbb{R}^N
\]

for the various values of \( \alpha \). Finally the saddle point expansion for the different cases yields the lemma.

An alternative way to study the large coupling limit is to perform it termwise in the HPE series of correlation functions. We specialize to the nearest neighbour interaction (19). The only way the coupling constants \( \lambda \) and \( \sigma \) enter the linked cluster expansion is via the connected one-point vertex couplings \( \tilde{v}^c_{2n} (\lambda, \sigma) \), defined in Eqn. (11). The connected one-point vertex couplings are related to the full one-point couplings \( \tilde{v}^{c}_{2n} \), defined by

\[
\tilde{v}^{c}_{2n} = \frac{\int d^N\Phi \tilde{v}^{c}_{2n} \exp (-S(\Phi))}{\int d^N\Phi \exp (-S(\Phi))},
\]

by the identity (12). At any finite order \( l \), the coefficient of \( \kappa^l \) is a polynomial in the \( \tilde{v}^{c}_{2n} \), hence in the \( \tilde{v}_{2n} \). Invoking a saddle point expansion again, we obtain
Lemma A.2 Let \( \lambda = \alpha \sigma \) with \( \sigma > 0, -\infty < \alpha < \infty \). Define for nonnegative integers \( N, k \)

\[
A_{N,k} = (2k - 1)!! \frac{\Gamma(\frac{N}{2})}{\Gamma(\frac{N}{2} + k)2^k}.
\]

As \( \sigma \to \infty \) we get for every \( k > 0 \)

\[\theta \]

\[\alpha > 1: \]

\[\theta \]

\[\alpha = 1: \]

\[\theta \]

\[\alpha = -3: \]

\[\theta \]

\[\alpha < -3: \]

\[\theta \]

For \( \alpha > 1 \) the vertices are identical with those of the O(N) Heisenberg models. In the range \( -3 < \alpha < 1 \) they agree with the vertices of a purely Gaussian model with ultralocal action

\[
\tilde{S}(\Phi) = (3 - 2\alpha)\sigma\Phi^2,
\]

leading to complete disorder as \( \sigma \to \infty \) for every finite \( \kappa \). For \( \alpha < -3 \) we obtain the Heisenberg model again, as can be seen as follows. For any \( \beta > 0 \), rescaling of the vertices

\[
\tilde{v}_{2k} \to \beta^{2k}\tilde{v}_{2k}
\]

implies a corresponding rescaling of the connected vertices, \( \tilde{v}_{2k}^c \to \beta^{2k}\tilde{v}_{2k}^c \), cf. (52). In turn, elementary graph theory shows that all susceptibilities change according to

\[
\chi_n(\kappa) \to \beta^n\chi_n(\beta^2\kappa).
\]

Hence, universality classes are invariant under (52). Furthermore we see that, for \( N \geq 2 \), the boundary points \( \alpha = 1 \) and \( \alpha = -3 \) belong to the Heisenberg class as well. A remnant of the occupation number variables is only seen in the case of \( N = 1 \), which is a remarkable exception and needs further study.

Thermodynamic quantities like \( \chi \) and the critical coupling \( \kappa_c \) can be directly determined in these limiting models. Alternatively, one may start with the original action (51) at finite \( \sigma \), calculate \( \chi \) and \( \kappa_c \) in the HPE, and take the large coupling limit last. Our results indicate that both limits commute.
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