Under quite general conditions critical phenomena can be described with high order linked cluster expansions. The coefficients of the series admit a graphical expansion that is generated with the aid of computers. Our generalization of linked cluster expansions from an infinite to a finite volume allows to perform a finite size scaling analysis. We also indicate a generalization to Dynamical Linked Cluster Expansions with possible applications to spin glasses and neural networks with coupled spin and interaction dynamics.

1 Linked Cluster Expansions in the Infinite Volume

We will focus on multiscale phenomena that occur as critical phenomena in statistical systems at second order phase transitions. We consider statistical systems with regions of first and second order transition regions in phase space. Our computational tools are analytical rather than numerical calculations. We use convergent series expansions in a parameter called hopping parameter $\kappa$. When applied to a calculation of the free energy and connected correlations, the expansions amount to Linked Cluster Expansions (LCEs). The expansion coefficients admit a representation as a sum of connected graphs. The price one has to pay for describing critical phenomena with an accuracy of the order of 1% is a high order in the expansion parameter. Since the number of contributing graphs rapidly increases with increasing order in $\kappa$, a computer aided algorithmic generation of graphs becomes unavoidable. Even an optimization...
of algorithms becomes essential to make the handling of millions of graphs feasible. Such a large number of graphs has to be dealt with to compute two and four-point functions to 20th order in $\kappa$ in LCEs. For example, this order is taken into account in scalar $O(N)$ models at finite temperature in order to measure the tiny finite temperature effects on the phase structure\cite{1}.

Originally, linked cluster expansions have been developed in the infinite volume. The reason why we have generalized them to a finite volume was twofold. One reason was to identify 1st order transitions from series expansions in the high temperature phase. The second reason was to distinguish second order transitions associated with different universality classes.

1.1 Algorithmic Generation of Graphs

A convenient representation of any graph $\Gamma$ is provided by an incidence matrix $I_{\Gamma}$ with matrix elements $I_{\Gamma}(i, j)$, $i, j \in 1 \ldots V$, $V$ being the number of vertices of $\Gamma$. Let us enumerate the vertices in some way. $I_{\Gamma}(i, j)$ is then given by

\begin{align}
I_{\Gamma}(i, i) &= \text{number of external lines at } v_i \\
I_{\Gamma}(i, j) &= \text{number of lines connecting vertices } v_i \text{ and } v_j, \quad i, j \in 1 \ldots V
\end{align}

This representation is not unique. For any permutation of vertices, $I_{\Gamma}$ will change unless it corresponds to a symmetry of $\Gamma$. A possible way out of this ambiguity is the introduction of a complete order relation among the $I$s. (For instance, $I^{(1)} > I^{(2)}$ if $(i', j')$ exists such that $I^{(1)}(i', j') > I^{(2)}(i', j')$, and $I^{(1)}(i, j) = I^{(2)}(i, j)$ for all $i = i'$, $j < j'$ and for all $i < i'$ and arbitrary $j$.) A unique representation of the graph is then defined as the maximum over all permutations of the vertices of $\Gamma$, i.e. as $I_{\Gamma}^{\text{max}} = \max_{\pi \in P_V} I_{\Gamma}^\pi$, where $I_{\Gamma}^\pi(i, j) = I_{\Gamma}(\pi(i), \pi(j))$. For the simple example of the graph of Fig. 1 $I_{\Gamma}$ and $I_{\Gamma}^{\text{max}}$ are given by

\begin{align}
I_{\Gamma} &= \begin{pmatrix} 1 & 1 & 0 & 2 \\ 0 & 1 & 0 \\ 1 & 2 \\ \cdots & 0 \end{pmatrix}, \\
I_{\Gamma}^{\text{max}} &= \begin{pmatrix} 1 & 2 & 1 & 0 \\ 0 & 0 & 2 \\ 0 & 1 \\ \cdots & 1 \end{pmatrix}.
\end{align}

Figure 1: Example for a graph with 2 external and 6 internal lines with labels attached to the vertices.
A CPU-time consuming part in computer aided LCEs is the complete and unique generation of graphs. It is performed iteratively with a certain algorithm for adding new lines and new vertices. It turns out that in order to make the algorithm both complete (i.e. generating all graphs that contribute) and efficient, multiple generations cannot be completely avoided. Let us assume that for a particular class of graphs we have just generated the \( n + 1 \)st graph after the first topologically inequivalent \( n \)'s have been generated. The time consuming procedure is then to find out whether the \( n + 1 \)st graph already exists among the first \( n \)s or not. One has to run through all \( \Gamma_i, i = 1, \ldots, n \) to decide whether \( \Gamma_{n+1} \) is topologically inequivalent to each of the first \( n \)s. A comparison between any 2 graphs is cheap if they are uniquely represented. If it is achieved via \( R^\text{max} \) as indicated above, \( V! \) permutations of vertices have to be performed for every newly generated graph to obtain this representation. This is quite a large number if one goes to a high order in the expansion parameter (for example it is 11! for the graph of order \( \kappa^{12} \) with 12 internal lines shown in Fig.2.)

To avoid the high factorials of permutations of incidence matrices, one needs a refined representation of graphs. One possibility is to first (partially) order the vertices and then to perform a maximization procedure. A vertex ordering that takes all local properties of vertices into account has been introduced by Lüsher and Weisz.3 With this improvement the 14th order in \( \kappa \) became feasible. A further refinement was an extended ordering proposed in1 which in addition accounts for nonlocal topological properties to distinguish vertices in combination with an iterated ordering. The type of ordering of vertices (if there is any) is reflected in the labelling of the vertices, cf. Fig. 2.

Figure 2: Different levels of ordering of vertices a. no ordering, b. according to 3, c. according to 1.

Fig. 2a shows a graph \( \Gamma \) with no labelling corresponding to no ordering, Fig. 2b with a ordering according to 3 and Fig. 2c with an extended ordering according to 1. The advantage now is that in order to define a final unique representation by means of the above maximization procedure, one has to perform permutations only among vertices with equal labels, this is 11! for Fig. 2a, 9! for Fig. 2b, but only \( 3!^3 \) for Fig. 2c. At best the number of
remaining permutations is as small as the symmetry factor of the graph, i.e. the number of simultaneous permutations of rows and columns that leave $I_T$ invariant. It turned out that the gain in CPU-time that is achieved because of the reduced number of permutations in $I$ is considerably larger than the loose because of the ordering of vertices. Further details on the (extended) ordering and the algorithmic performance can be found in [1].

2 The Monotony Criterion and its Application to Monte Carlo Simulations

In LCEs the action is split into a sum of ultralocal parts $\hat{S}$ and a next neighbour part $S_{nn}$ with next neighbour couplings $\propto \kappa$. A Taylor expansion in $\kappa$ of the logarithm of the partition function $\ln Z$ about the ultralocal contribution to $\ln Z$ finally leads to graphical expansions of $n$-point susceptibilities $\chi_n$ with coefficients $a_\mu^{(n)}$. For every $\mu$, $n$, $a_\mu^{(n)}$ is a sum over all connected graphs with $\mu$ internal and $n$ external lines each of which adds as its weight a product of the inverse topological symmetry factor, an internal symmetry factor, a lattice embedding factor, and a product of vertex contributions depending on the couplings involved in $\hat{S}$. It is only the embedding factor that depends on the topology of the particular lattice that will change in passing from an infinite to a finite volume.

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 has to be further specified. For definiteness we fix the notation in terms of order parameter susceptibilities $\chi$. In particular, at $T_c(V)$, $\chi$ 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 in the finite volume. In [2] we have made these statements more precise in order to show that the monotony behaviour of the susceptibilities is neither a peculiarity of specific models nor an artifact of the series expansion. It is a generic feature of models with first and second order transitions if the standard assumptions on their finite size scaling behaviour apply. Here we further comment on applications to Monte Carlo calculations.

Choose two volumes $V_1$, $V_2$ both sufficiently large in order to satisfy the standard assumptions of a FSS so that the regular contribution to $\chi$ and its
induced generic volume dependence are negligible. Let $V_1 \ll V_2$ as argued below. Let $\lambda$ denote a generic coupling parametrizing the transition surface in coupling constant space. Choose $\delta$ such that $c_1 \sigma(V_2) \frac{\epsilon}{\delta^2} < |\delta| < c_2 \sigma(V_1)$, where $c_1$, $c_2$ and $\epsilon$ are positive constants and $\sigma$ denotes the width of the critical region. Define

$$r_{V_1,V_2} := 1 - \frac{\chi_2(\delta + \kappa_c(V_1), V_1)}{\chi_2(\delta + \kappa_c(V_2), V_2)}.$$  

(4)

The monotony criterion says that

$$r_{V_1,V_2} \begin{cases} > 0, & \text{2nd order} \\ < 0, & \text{1st order} \\ = 0, & \text{tricritical point for } \partial r/\partial \lambda \neq 0. \end{cases}$$  

(5)

The difference of using the monotony criterion in Monte Carlo simulations or in series representations of $\chi$ comes from the second volume $V_2 > V_1$ that must be finite in Monte Carlo simulations, but can be infinite in LCEs. For $V_2 < \infty$ also in case of 1st order transitions a small neighbourhood around the peak of $\chi$ exists where $\chi$ increases with $V$ because of the rounding of the $\delta$-singularity. Thus $V_2$ should be chosen sufficiently larger than $V_1$ so that the widths of the critical regions behave like $\sigma(V_2) \ll \sigma(V_1)$. For finite $\sigma(V_2)$ the points $T$ or $\kappa$ at which the $\chi$s are evaluated should be chosen at the same distance from the (volume dependent) position of the peak of $\chi$.

Deviations from these predictions in Monte Carlo calculations may be caused by

- $V_1, V_2$ both too small
- $V_2/V_1$ too small
- $(\kappa - \kappa_c(V))/\kappa_c(V)$ too large, i.e. contributions from the regular part cannot be neglected.
- $(\kappa - \kappa_c(V))/\kappa_c(V)$ too small, so that $r > 0$ even for 1st order.

In particular the interval of allowed $\kappa$s in Eq. (5) depends on the coupling $\lambda$. Note that the ratios of Eq. (4) do not include the generic volume dependence that is induced by the analytic part of $\chi$. Assuming that one is lucky in simultaneously matching these constraints, a result of $r_{V_1,V_2} > (<) 0$ for all $\kappa$ from the specified scaling region excludes (indicates) a 1st order transition, respectively.

If there is a crossover phenomenon rather than a true phase transition, $r$ should vanish for a finite neighbourhood of $\lambda$ for sufficiently large $V_1, V_2$.

An application of the monotony criterion to LCEs in a scalar $O(N)$ theory with $\Phi^4$ and $\Phi^6$-terms in 3 dimensions with $N = 1$ or $N = 4$ improved the localizability of the tricritical line in this model by 2 orders of magnitude.
Dynamical Linked Cluster Expansions

As Dynamical Linked Cluster Expansions (DLCEs) we call LCEs with dynamical next neighbour couplings. The next neighbour couplings still play the role of expansion parameters, but are endowed with their own dynamics. More precisely DLCEs amount to the following generalization of the familiar linked cluster expansions.

Let \( \Lambda \) denote the set of sites of a hypercubic lattice, \( \frac{1}{2} \Lambda \) the set of unordered pairs of sites \( l = (xy) \), not necessarily nearest neighbours. We consider a statistical system characterized by the partition function

\[
Z(H, J; v) = \mathcal{N} \int \prod_{x \in \Lambda} d\Phi_x \cdot \prod_{l \in \Lambda} dU_l \cdot \exp \left[ -S(\Phi, U; v) + \sum_{x \in \Lambda} H_x \Phi_x + \sum_{l \in \Lambda} J_l U_l \right]
\]

with normalization factor \( \mathcal{N} \) such that \( Z(0, 0, v) = 1 \) and an action \( S \) having the form

\[
S(\Phi, U; v) = \sum_{x \in \Lambda} ^0 S(\Phi_x) + \sum_{l \in \Lambda} ^1 S(U_l) - \frac{1}{2} \sum_{x,y \in \Lambda} v_{xy} \Phi_x U_{(xy)} \Phi_y
\]

with \( v_{xy} = v_{yx}, v_{xx} = 0 \). \( \Phi \) can be an \( N \)-component scalar field associated with the lattice sites \( x \) or a \( Z_N \)-spin, likely \( U \) can be any scalar, vector or tensor field associated with lattice links \( l \). The action \( S \) is split into two ultralocal parts \( ^0 S \) and \( ^1 S \), depending on single sites and on single links via the fields \( \Phi_x \) and \( U_l \), and an interaction part with coupling constants \( v_{xy} \). Note that formally the former coupling \( v_{xy} \) is replaced by \( v_{xy} \cdot U_{xy} \) with the dynamics of \( U \) governed by \( ^1 S \).

A new type of graphical expansion of \( n \)-point correlation functions is then induced by Taylor expanding \( \ln Z(H, J; v) \equiv W(H, J; v) \) about \( v = 0 \) with

\[
W(H, J; v = 0) = \sum_{x \in \Lambda} ^0 W(H) + \sum_{l \in \Lambda} ^1 W(J).
\]

To illustrate the new features, we list the terms occurring in the second derivatives in the Taylor expansion of \( W \). Written as indices, let \( J_{(lm)} \) and \( H_l \) stand for the derivatives of \( W \) with respect to \( J_{(lm)} \) and \( H_l \) at \( v = 0 \), respectively. The expressions

\[
W_{H_j} \cdot W_{J_{ij}} \cdot W_{H_l} \cdot W_{H_m} \cdot W_{J_{lm}}
\]
suggest a graphical representation according to Fig. 3, respectively.

\[
W_{J_{ij}} \cdot W_{H_{H_{i}}} \cdot W_{H_{m}} \cdot W_{H_{j}} \cdot W_{J_{ij}} \\
W_{H_{H_{i}}} \cdot W_{H_{m}} \cdot W_{H_{j}} \cdot W_{J_{ij}} \\
W_{H_{j}} \cdot W_{H_{i}} \cdot W_{H_{m}} \cdot W_{J_{ij}} \\
W_{H_{i}} \cdot W_{H_{j}} \cdot W_{H_{m}} \cdot W_{J_{ij}} \\
\] (9)

The dashed lines indicate the new type of local connectivity, originating from \( W \), \( n \) lines are now connected if at least one of the following conditions is met.

- The lines share a common vertex \( v_n \equiv \frac{\partial W^0}{\partial H^n} \) as before.
- The lines are part of a multiple-line sharing a common factor \( g_n \equiv \frac{\partial^0 W}{\partial J^n} \).

Thus the building blocks of the graphical expansion for DLCEs are \( m \)-point vertices and \( n \)-multiple-lines as shown in Fig. 4.

Figure 3: Graphical representation of the terms of Eq. (9), respectively.

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Figure 4: Graphical rules for DLCEs.

Note that the graphs of the former LCEs are contained as a small subclass of the graphs of DLCEs. If we replace for constant \( U \cdot v U \) by \( v \) and choose \( W(\cdot J) \) as \( J_1 \cdot v \), we have \( \frac{\partial W}{\partial J} = v \) (1-lines as before), but \( \frac{\partial W}{\partial J_n} = 0 \) for \( n > 1 \) (corresponding to no multiple-lines).

A rapid increase in the number of graphs contributing to an \( n \)-point susceptibility sets in at low order in the expansion in \( \kappa \). For example the number of graphs contributing to \( \chi_2 \) to order \( \kappa^4 \) is of the order of 100, while it is by an order of magnitude smaller in the pure LCE of \( \chi_2 \).
The generic form for the action in Eq. (7) has interesting physical applications to systems with coupled dynamics with (fast) spins and (slow) interactions in spin glasses and neural networks, in which both spins and couplings are endowed with a dynamical law and evolve in time.

So far the graphs for LCEs could be generated on a SUN-workstation with a CPU-time of the order of days and a working space of the order of 100 MB. Work on computer aided DLCEs is in progress.

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