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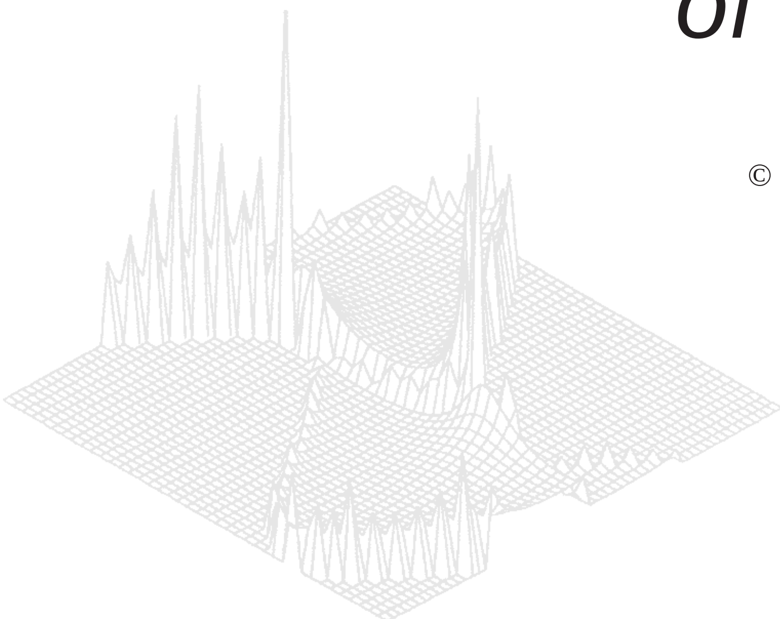

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Finite-Size Scaling and Effective Lagrangian Theory*

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Abstract

A brief review is given of the 'effective Lagrangian' approach of Leutwyler, Hasenfratz and others, which describes the behaviour at low energies or temperatures, or large distances, in lattice systems which undergo a first-order transition involving spontaneous breakdown of a continuous symmetry. Universal predictions can be given, based on a continuum field theory of the massless Goldstone bosons generated by the breakdown of the symmetry, which control the behaviour in these regimes. In particular, the finite-size scaling behaviour can be predicted, in a way very similar to the predictions of conformal invariance for a two-dimensional system at a critical point. Conversely, measurements of the finite-size scaling behaviour can give estimates of the parameters of the Goldstone bosons. These points are illustrated using data for the O(2) Heisenberg spin model in (2+1) dimensions, and the XXZ antiferromagnet on a square lattice.

1. Introduction

For the past twenty or thirty years, there has been an extremely fruitful exchange of ideas between the disciplines of quantum field theory and statistical mechanics. This has stemmed partly from the recognition that the 'generating functionals' in both cases, namely the Feynman path integral on one hand and the partition function on the other, are essentially equivalent mathematical objects. Physically, it also stems from the fact that when a lattice system is at a second or higher order critical point, the correlation length diverges, fluctuations occur on all length scales, and the microscopic details of the lattice become unimportant. The behaviour of the system at large distances or low energies is then dominated by the lowest mass excitations of the system, which can be described by a continuum field theory. In this paper we will be particularly interested in lattice spin models of magnetic systems, such as the Heisenberg model. We will also restrict our attention to phenomena in the neighbourhood of a phase transition, where most of the physical interest lies.

From the basis above, there has sprung a succession of important theoretical concepts:

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(1) Scale invariance and universality (Kadanoff, Fisher *et al.*);
(2) The renormalisation group (Wilson);
(3) Conformal invariance (Polyakov *et al.*);
(4) The 'effective Lagrangian' approach (Hasenfratz and Leutwyler 1990; Hasenfratz and Niedermayer 1993), which will be the subject of the present paper.

The arguments and results which we shall review can apply almost unchanged to *either* a classical spin model at a critical temperature, or to a quantum spin model at a critical value of the coupling constant, provided we make the following correspondences (Barber 1983):

Classical spin model, $T = T_c$ (d dimensions)	Quantum spin model, $T = 0$, $J = J_c$ (1 time, $d{-}1$ space dimensions)
Partition function	Feynman path integral
Thermal fluctuations	Quantum fluctuations
Correlation length	Inverse mass gap
log[transfer matrix]	Quantum Hamiltonian
Free energy	Ground state energy
e.g. classical O(N) Heisenberg ferromagnet	e.g. $S = \frac{1}{2}$ Heisenberg AF

2. Finite-size Scaling

The theory of finite-size scaling, as formulated originally by Fisher (1972), Barber (1983) and others, concerns the way in which the behaviour of a system of finite size approaches its bulk limit. Heuristically, the argument runs that in the neighbourhood of a critical point, there is only one scale that matters in the problem, set by the correlation length ξ. In that neighbourhood we expect the correlation length to diverge as

$$\xi \sim (T - T_c)^{-\nu}; \quad T \to T_c \,, \tag{1}$$

while for instance the susceptibility is

$$\chi \sim (T - T_c)^{-\gamma} \sim \xi^{\gamma/\nu} \,. \tag{2}$$

But for a finite system of size L, the correlation length cannot be greater than the size of the system. Thus we expect at the critical point

$$\xi \sim L, \quad L \to \infty \tag{3}$$

or the mass gap

$$m \sim 1/L \tag{4}$$

and

$$\chi \sim \xi^{\gamma/\nu} \sim L^{\gamma/\nu} \,. \tag{5}$$

These arguments were placed on a more systematic footing by Suzuki (1977) and Brézin (1982), using the renormalisation group.

Now these observations are not of much use experimentally, because hardly any physical systems are *small* enough for the finite-size corrections to be visible. They turned out to be of great importance theoretically, however, because:

- Most numerical methods of calculation, such as exact diagonalisation (Lanczos), Monte Carlo simulations, or density-matrix renormalisation group calculations, for example, give results for finite systems only. Finite-size scaling theory tells us what the expected finite-size corrections are, and how the finite-lattice results may be scaled or extrapolated to the bulk limit.
- Also, the finite-size scaling behaviour (3)–(5) can be *exploited* to obtain accurate estimates of the critical parameters (Barber 1983; Nightingale 1977; Nightingale and Blote 1980; Hamer and Barber 1980, 1981). An example appears in Table 1. This has become a large theoretical industry in recent years.

Table 1. Sequence approximants to the critical index $1/\nu$ for the $\mathbf{Z}_3$ spin model in (1+1) dimensions (Hamer and Barber 1981)

The left-hand column lists 'raw' values obtained from lattices of 2,3,.., 10 sites, and the other columns list successive extrapolations of the finite-lattice sequence to the bulk limit, obtained using a VBS algorithm. The expected exact value is $1\cdot 2$

1·723515				
1·476662	1·341853			
1·389470	1·295290	1·200474		
1·344194	1·271839	1·200392	1·200593	
1·316345	1·257646	1·200252	1·199889	1·2000015
1·297457	1·248115	1·200151	1·200156	
1·283798	1·241267	1·200156		
1·273459	1·236109			
1·265362				

3. Conformal Invariance

The scaling hypothesis states that a critical system is 'self-similar' (or scale invariant) at all distance scales; for instance, correlation functions behave as

$$G(r) \sim \frac{1}{r^{2-d+\eta}}, \quad r \to \infty\,, \tag{6}$$

so that

$$G(br) \sim b^{-(2-d+\eta)} G(r)\,, \tag{7}$$

or in other words the correlation function is *covariant* under scale transformations.

Polyakov (1970) generalised the hypothesis of scale invariance to include conformal invariance, and boldly conjectured that this might actually *determine* the critical exponents (on the general principle that increased symmetry implies increased constraints on the system). Belavin *et al.* (1984) and Friedan *et* *al.* (1984) showed that this program actually *works* in the special case of two dimensions:

- The conformal group in two dimensions includes local rescalings and rotations without shear (i.e. preserving angles). Uniform rescalings are a sub-group. Field theories containing only dimensionless coupling parameters *are* conformal invariant, unless the symmetry is 'spontaneously broken'. Maxwell's equations provide a well-known example.
- There exists an associated 'Virasoro algebra' involving a constant c called the 'central charge' or 'conformal anomaly'. Each theory is characterised by its value of c, and all the critical exponents are related to it.
- If $c < 1$, the critical exponents lie in a discrete set, labelled by an *integer* $m \geq 3$, due to the requirement of unitarity (or reflection positivity):

$$c = 1 - \frac{6}{m(m+1)}, \quad m = 3, 4, 5, ... \tag{8}$$

- The asymptotic behaviour of all correlation functions is determined by conformal invariance.

Conformal invariance has important implications for the finite-size scaling properties of the system, as shown by Cardy (1987, 1988) and Christe and Henkel (1993). It turns out that the finite-size scaling *amplitudes* at the critical point are *universal* numbers, related to the scaling indices; e.g. for a quantum Hamiltonian system of size L in $(1{+}1)D$, with periodic boundary conditions, one finds that the ground-state energy per site behaves as (Affleck 1986; Blote *et al.* 1986):

$$\epsilon_0(L) - \epsilon_0(\infty) \sim -\frac{\pi c v}{6L^2}, \quad L \to \infty\,, \tag{9}$$

where v is the spin-wave velocity, or 'speed of light'. Hence the conformal anomaly c can be determined. An example is shown in Fig. 1.

The mass gaps behave as (Cardy 1984):

$$E_i - E_0 \sim \frac{2\pi x_i v}{L}\,, \tag{10}$$

where x_i is the corresponding *scaling index*. An example is shown in Fig. 2.

Measurement of these finite-size scaling amplitudes thus provides a powerful tool for estimating the scaling indices x_i, and fixing the universality class of the system. The finite-lattice eigenvalue spectrum in fact forms a *representation* of the conformal group.

This is all very fine in two dimensions; but what about *higher* dimensions? Some limited results have recently become available, as we shall see below.

4. Effective Lagrangian Theory

At a *first-order* transition, in a model with a *continuous symmetry group*, in dimension $d > 2$, we expect that:

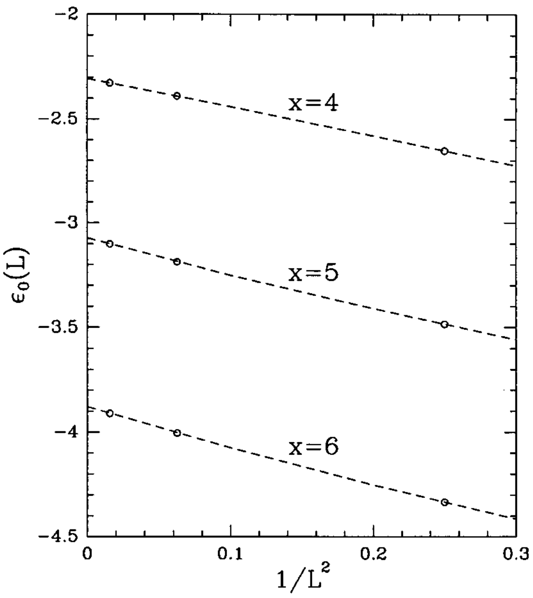

Fig. 1. Ground-state energy density ϵ_0 for the O(2) quantum spin model in (1+1)D, plotted as a function of $1/L^2$, where L is the lattice size, for various couplings x. Straight line fits are shown (Wang and Hamer 1993). This model has a critical line at large x.

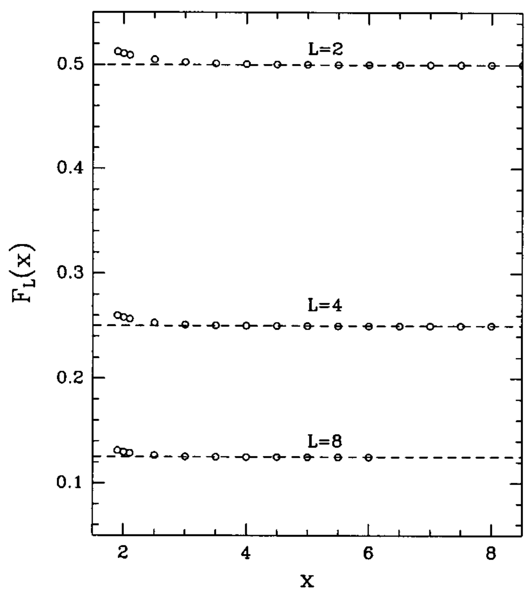

Fig. 2. Finite-lattice mass gap for the O(2) model in (1+1)D, plotted as a function of coupling x for various lattice sizes L (Wang and Hamer 1993). It can be seen that at large x the mass gap is almost precisely equal to $1/L$, indicating critical behaviour.

- The symmetry is spontaneously broken;
- The system develops *Goldstone bosons* (Goldstone's theorem).

An example is the famous 'Mexican hat potential'. If an underlying O(2) symmetry is spontaneously broken, one Goldstone mode is developed; for the case with O(3) symmetry, two Goldstone modes are developed; and for O(N) symmetry, ($N-1$) Goldstone modes occur. These are simply the 'magnons' or spin-waves of the theory.

The 'effective Lagrangian' hypothesis (Hasenfratz and Leutwyler 1990; Hasenfratz and Niedermayer 1993) postulates that the behaviour of the system at large distances and low energies is that of an effective continuum field theory of massless Goldstone bosons. One can write an effective Lagrangian for the Goldstone bosons, which respects the original symmetry of the theory; and hence develop a systematic large-volume or low-energy expansion, which gives *universal formulae* for the leading finite-size corrections (and also the leading low temperature or low field corrections), in terms of a few unknown parameters characteristic of the Goldstone bosons. This situation is very reminiscent of the conformal invariance results in two dimensions. The effective theory is generally infrared convergent, but ultraviolet divergent and non-renormalisable; this does not affect its ability to provide a systematic expansion at large sizes or volumes. This approach had its origins in chiral perturbation theory in QCD, where low-energy effects can be described in terms of low-mass pi-mesons and other pseudo-Goldstone excitations: the true underlying theory is presumably QCD itself, a renormalisable theory of quarks and gluons, but the effective pion theory is more useful for describing certain classes of low-energy or long-distance phenomena.

Predictions

(A) Models with O(N) symmetry, in $d > 2$*, e.g. the classical Heisenberg ferromagnet*

In the first-order transition region, a finite-size or large-volume expansion is obtained in powers of $1/L^{d-2}$ (where the volume $V = L^d$). The parameters involved are the spin-wave helicity modulus or spin-wave stiffness

$$\rho_s = \Upsilon\,, \tag{11}$$

and the bulk magnetisation per spin in the bulk Σ. The effective Lagrangian density is

$$L_{eff} = \tfrac{1}{2}\rho_s(\partial_\mu \mathbf{S}.\partial_\mu \mathbf{S}) - \Sigma(\mathbf{H}.\mathbf{S}) + ... \quad (\mathbf{S}.\mathbf{S} = 1)\,. \tag{12}$$

The predictions obtained include the magnetisation for a small magnetic field:

$$M_H(V) \to \frac{1}{N}\Sigma^2 HV\rho^2, \quad H \to 0\,, \tag{13}$$

$$\rho = 1 + \frac{(N-1)\beta_1}{2\rho_s L^{d-2}} + O(L^{2d-4})\,, \tag{14}$$

and the susceptibility

$$\chi_{\parallel}(H{=}0,V) = \frac{V\Sigma^2}{N} + \frac{L^2(N-1)\Sigma^2\beta_1}{N\rho_s} + O(L^{4-d}) \tag{15}$$

(β_1 is a geometrical structure constant with value $0{\cdot}226$ in $d = 3$). These predictions have been nicely confirmed by the numerical calculations of Dimitrovic *et al.* (1991), for the case of the O(3) Heisenberg model in three dimensions.

(B) The $S = \frac{1}{2}$ quantum Heisenberg antiferromagnet at $T = 0$ on a square lattice.

Here the quantum Hamiltonian is

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i.\mathbf{S}_j\,. \tag{16}$$

The terms in the Hamiltonian do not commute, and quantum fluctuations occur. The Hamiltonian possesses rotational O(3) symmetry, which is spontaneously broken. The model has been much studied recently, because of its possible connections with high-T_c superconductivity. Hasenfratz and Niedermayer (1993) have made a number of predictions for the finite-size corrections in this model, and its behaviour at low temperatures and small magnetic field. The parameters are the helicity modulus ρ_s, the spin-wave velocity v, and the magnetisation per unit volume Σ. These are not predicted by the theory. The effective Lagrangian density is a slight generalisation of the previous one:

$$L_{eff} = \tfrac{1}{2}\rho_s\left[\frac{1}{v^2}\partial_t\mathbf{S}.\partial_t\mathbf{S} + \sum_{i=1,2}\partial_i\mathbf{S}.\partial_i\mathbf{S}\right] - \Sigma(\mathbf{H}.\mathbf{S}) + ... \quad (\mathbf{S}.\mathbf{S} = 1)\,, \tag{17}$$

to allow for space–time anisotropy. For the more general case with O(N) symmetry, the following predictions are obtained.

Predictions

(1) Low-temperature corrections ($T \neq 0, V \to \infty$)

Correlation length:

$$\xi(T) = \frac{ev\mathrm{e}^{2\pi\rho_s/T}}{16\pi\rho_s}\left[1 - \frac{T}{4\pi\rho_s} + O(T^2)\right]. \tag{18}$$

Specific heat:

$$C(T) = (N-1)\frac{3\zeta(3)}{\pi v^2}T^2 + O(T^4) \quad [\zeta(3) = 1{\cdot}2020...]\,, \tag{19}$$

arising from the free energy of $N{-}1$ massless, free bosons (where $N = 3$ for the XXZ antiferromagnet). The predicted behaviour of the correlation length agrees very well with experimental data (e.g. Greven *et al.* 1994).

(2) Finite-size corrections ($T = 0$, finite L)

Ground-state energy per site:

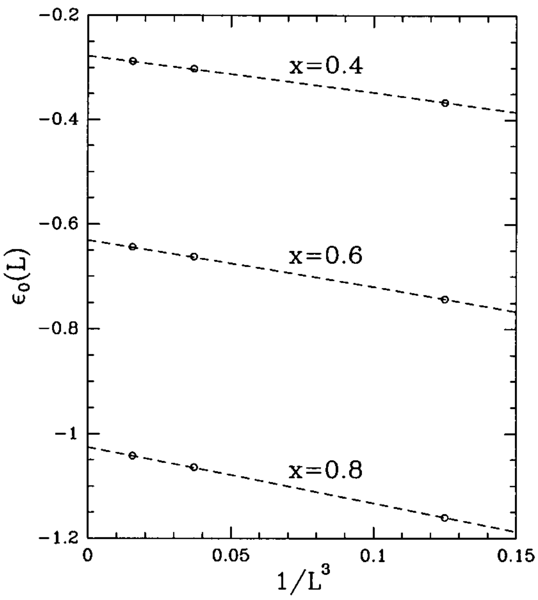

Fig. 3. Ground-state energy density of the O(2) quantum spin model in (2+1)D (Wang and Hamer 1993), plotted as a function of $1/L^3$ for various couplings x. Straight line fits are shown. This model has a first-order transition line at large x.

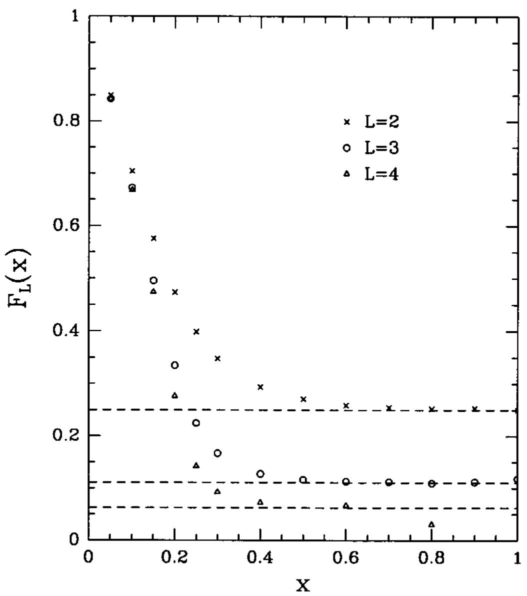

Fig. 4. Finite-lattice mass gap of the O(2) model in (2+1)D, plotted as a function of x for various lattice sizes L (Wang and Hamer 1993). It can be seen that the mass gap is almost equal to $1/L^2$ at large x, in agreement with effective Lagrangian theory.

$$\epsilon_0(L) - \epsilon_0(\infty) = -\frac{(N-1)1\cdot 4377...v}{2L^3} + \frac{(N-1)(N-2)v^2}{8\rho_s L^4} + ... \qquad (20)$$

Mass gaps:

$$E_j - E_0 = \frac{j(j+N-2)v^2}{2\rho_s L^2}\left[1 - \frac{(N-2)v}{\rho_s L}\frac{3\cdot 9003}{4\pi} + ...\right]. \qquad (21)$$

The leading terms in these expansions were previously obtained by Neuberger and Ziman (1989), and Fisher (1989). These predictions are in excellent agreement with numerical Monte Carlo data for the XXZ Heisenberg antiferromagnet (Runge 1992), and the quantum Hamiltonian version of the classical O(2) spin model (Wang and Hamer 1993) — see Figs 3 and 4.

The values of ρ_s, v and Σ are not predicted by the effective Lagrangian approach, but they can be estimated using the spin-wave expansion of Anderson and Kubo, applied to the original Hamiltonian. These approaches are of course compatible, since both involve spin waves or magnons (Zheng and Hamer 1993; Hamer *et al.* 1992). A comparison between the values obtained from the theoretical spin-wave expansion, and from numerical Monte Carlo and series calculations for the XXZ model on the square lattice is shown below. It can be seen that the different estimates generally agree very well, and thus provide strong confirmation of the theoretical scenario above.

Quantity	Spin-wave expansion[A]	Monte Carlo[B]	Series[C]
$\epsilon_0(\infty)/J$	$-0\cdot 670$	$-0\cdot 66934(3)$	$-0\cdot 6694(1)$
Σ	$0\cdot 307$	$0\cdot 3075(25)$	$0\cdot 307(1)$
ρ_s	$0\cdot 175$	$0\cdot 199(2)$	$0\cdot 182(5)$
v	$1\cdot 67$	$1\cdot 55(4)$	$1\cdot 655(12)$

[A] Zheng *et al.* (1991), Zheng and Hamer (1993), Hamer *et al.* (1992, 1994), Igarashi (1992) and Canali *et al.* (1992).
[B] Runge (1992) and Makivic and Ding (1991).
[C] Zheng *et al.* (1991), Hamer *et al.* (1992), Singh (1989) and Singh and Huse (1989).

5. Conclusions

In higher dimensions ($d > 2$), for first-order transitions in models with spontaneous breakdown of a continuous symmetry, finite-size scaling again provides a powerful tool for extracting parameters of the effective continuum field theory. Universal forms again emerge from the effective Lagrangian approach, although the parameters involved are ρ_s, v and Σ, for instance, rather than scaling dimensions.

One is left with the final question: what is the finite-size scaling behaviour at a *second-order* transition in higher dimensions; and what can it tell us about the effective field theory at the transition?

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