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Finite-lattice methods in quantum Hamiltonian field theory: II. O(2) and O(3) Heisenberg models

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Abstract. Two efficient methods for finding the low-lying states of Hamiltonians on finite lattices are described. The first involves constructing a finite representation of the Hamiltonian using strong-coupling eigenstates, while the second is based on the Lanczos recursion method. The methods are used to determine the mass gap of the O(2) and O(3) Heisenberg Hamiltonians in $(1+1)$ dimensions for a sequence of finite chains. The critical behaviour of the infinite chain is then analysed by extrapolating the finite-lattice estimates using finite-size scaling. A remarkably sensitive test is developed for the presence of a phase transition. For the O(2) model data this test yields strong evidence for a phase transition with the weak-coupling phase massless, while in the O(3) case the test supports, although more weakly, the absence of any transition.

1. Introduction

In the preceding paper (Hamer and Barber 1981), hereafter referred to as I, we discussed the behaviour of the Hamiltonian version of the two-dimensional Ising model using finite-size scaling. Our primary interest was not in this model in itself, but in the feasibility of extracting the behaviour of the theory from the way in which physical quantities varied with the size of the lattice. The results reported in I indicated that this approach was quantitatively as accurate as series methods (see e.g. Hamer and Kogut 1979). In this paper we extend our techniques to investigate the Hamiltonian versions of O(N) Heisenberg models ($N=2, 3$) in $(1+1)$ dimensions. A preliminary announcement of some of these results has already been given (Hamer and Barber 1980).

The Hamiltonian field theory versions of these models have been discussed by Hamer *et al* (1979). The lattice Hamiltonian takes the form

$$H=\frac{g}{2a}\sum_{m=1}^{M}[\boldsymbol{J}^2(m)-x\boldsymbol{n}(m)\cdot\boldsymbol{n}(m+1)], \tag{1.1}$$

where the sum runs over the M sites of a chain with periodic boundary conditions. In addition, g is a dimensionless coupling, a is the lattice spacing, $x=2/g^2$, $\boldsymbol{J}(m)$ is the angular momentum operator appropriate to the O(N) rotational symmetry, and $\boldsymbol{n}(m)$ is an N-component spin vector normalised to unity.

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These Hamiltonians differ from the Ising Hamiltonian treated in I in two features. Firstly, it does not appear possible to diagonalise them analytically, even for finite M. Secondly, and rather more significantly, the state space of the Hamiltonian is infinite even on a finite chain. Thus in a numerical approach we cannot hope to calculate eigenvalues exactly, but must resort to a numerical procedure which hopefully yields sufficiently accurate numbers for a reasonable degree of computation.

In § 2 we describe two methods which appear to satisfy this criterion. In essence, the first method uses strong-coupling eigenstates to construct a finite-matrix representation of H. This matrix can then be diagonalised by standard procedures. The second is a recursive method based on the Lanczos method of tri-diagonalisation. The remainder of the paper is arranged as follows. Section 3 describes the analysis of the O(2) mass gap results for the existence of a scale-invariant region. To do this we make use of a refinement of phenomenological renormalisation (Nightingale 1977, Sneddon and Stinchcombe 1979, described in Hamer and Barber 1980). The nature of the singularity at the terminus of this scale-invariant region (the analogue of the Kosterlitz–Thouless point) is also discussed. Section 4 is devoted to the O(3) model, which supplies a further test of our method for two reasons. It is a non-Abelian model and is expected not to exhibit a phase transition. Section 5 contains some calculations and comments pertaining to the weak-coupling regime of the O(2) Hamiltonian on a finite chain. Section 6 closes the paper with an overall summary and discussion.

2. Method

For simplicity we describe our methods of diagonalising finite-lattice Hamiltonians by reference to the Ising Hamiltonian

$$H = \frac{g}{2a} \sum_{m=1}^{M} [1 - \sigma_3(m) - x\sigma_1(m)\sigma_1(m+1)], \tag{2.1}$$

where $\sigma_i(m)$ are Pauli spin matrices and the notation is otherwise as before. Let us write this Hamiltonian as

$$H = (g/2a)W, \qquad W = W_0 - xV, \tag{2.2}$$

where

$$W_0 = \sum_{m=1}^{M} [1 - \sigma_3(m)] \tag{2.3}$$

and

$$V = \sum_{m=1}^{M} \sigma_1(m)\sigma_1(m+1). \tag{2.4}$$

2.1. Strong-coupling eigenstate method

The essential idea (Hamer 1979) of this first method is to generate a set of strong-coupling eigenstates of W_0 by successive applications of the operator V to an unperturbed eigenstate of W_0. The assumption of periodic boundary conditions means that we may restrict ourselves to periodic states.

Let us outline explicitly the calculation of the ground state of W for a lattice of size $M = 5$. The ground state of H_0 is the state $|0\rangle$ such that

$$\sigma_3(m)|0\rangle = |0\rangle \qquad \text{for all } m. \tag{2.5}$$

We represent this state by an empty chain:

$$|0\rangle = |\,.\,.\,.\,.\,.\,\rangle. \tag{2.6}$$

Application of V gives a state

$$|1\rangle = \frac{1}{\sqrt{5}}\Big(|\,|\,|\,.\,.\,.\,\rangle + |\,.\,|\,|\,.\,.\,\rangle + |\,.\,.\,|\,|\,.\,\rangle + |\,.\,.\,.\,|\,|\,\rangle + |\,|\,.\,.\,.\,|\,\rangle\Big) \tag{2.7}$$

where a bar '|' denotes a flipped spin. We shall denote $|1\rangle$ simply by $|\,|\,|\,\rangle$, where the translational invariance is implicit. Application of V to $|\,|\,|\,\rangle$ now gives a combination of two eigenstates of H_0:

$$V|\,|\,|\,\rangle = 2(|\,|\,.\,|\,\rangle + |\,|\,|\,|\,|\,\rangle) + \sqrt{5}|0\rangle, \tag{2.8}$$

where the periodic extension of each state is understood. Thus we now have a four-dimensional basis consisting of $|0\rangle$, $|1\rangle$ and two new states:

$$|2\rangle = |\,|\,.\,|\,\rangle, \qquad |3\rangle = |\,|\,|\,|\,|\,\rangle. \tag{2.9}$$

Reapplication of V to these states generates no new states. This is of course a special feature of the Ising system and reflects the fact that this Hamiltonian has a finite state space. For the O(N) model this procedure does not terminate, but as we shall see converges rather rapidly.

Using the basis $\{|n\rangle, n = 0, 1, 2, 3\}$ we now form the matrix $\langle n|H|m\rangle$, which is given explicitly by

$$\begin{pmatrix} 0 & -x\sqrt{5} & 0 & 0 \\ -x\sqrt{5} & 4 & -2x & -2x \\ 0 & -2x & 4-2x & -x \\ 0 & -2x & -x & 8-2x \end{pmatrix}. \tag{2.10}$$

The lowest eigenvalue of this matrix is

$$\omega_0 = 4 - x - 2[1 + x^2 + 2x\cos(2\pi/5)]^{1/2} - 2[1 + x^2 + 2x\cos(4\pi/5)]^{1/2},$$

which agrees with that obtained in I analytically.

To obtain the energy of the first excited state of H we repeat the process, but start from the first excited state of H_0, which consists of a single flipped spin.

This method can be easily extended (Hamer *et al* 1979) to the O(N) models with

$$W_0 = \sum_m \boldsymbol{J}^2(m) \tag{2.11}$$

and

$$V = \sum_m \boldsymbol{n}(m) \cdot \boldsymbol{n}(m+1). \tag{2.12}$$

The only important new feature is that the operator $\boldsymbol{J}^2(m)$ now has an infinite spectrum of eigenvalues, whereas in the Ising model there were only two. Therefore the complete set of eigenstates on the finite lattice is no longer finite, and it is no longer possible to

compute the exact eigenvalues of H by exhausting the state space by successive applications of V.

Nevertheless, sufficiently precise results may be obtained by perturbing to high enough orders. This is illustrated in figure 1, which shows approximations to the mass gap $F(x)$ for the O(2) model on a 3-site lattice, obtained at various orders N. It can be seen that the successive estimates converge very rapidly at any fixed value of x and 'map out' the function $F(x, M)$ over successively larger regions. Except in the very-large-x regime, one may get sufficiently accurate estimates of $F(x, M)$ by perturbing to order $N \sim \mathrm{O}(M)$. In this manner we have been able to evaluate the ground state and first excited states of (1.1) for $M \leqslant 6$. It should be noted that technically this calculation is similar to the strong-coupling expansions, but carried to higher order. In the strong-coupling expansions (Hamer *et al* 1979) the perturbation coefficients were obtained by taking a finite lattice of M sites (M odd) and perturbing to order $(M-1)/2$. To this order the finite-lattice estimate and the exact *infinite*-lattice energies agree when expanded in powers of x.

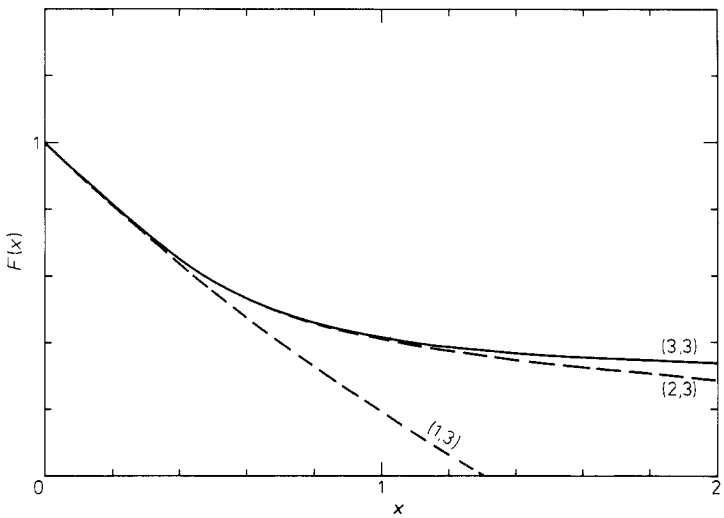

Figure 1. Mass gap of the O(2) Hamiltonian on a 3-site lattice. The broken curves are finite-order approximations, labelled (N, M), where $M = 3$ is the number of sites and N is the order in perturbation. The full curve is the limiting 'exact' result obtained for $N \geqslant 3$.

2.2. Recursive method

An alternative method we have investigated to some extent is based on recursive methods similar to those used in band theory (see e.g. Haydock *et al* 1975) and nuclear physics (see e.g. Whitehead *et al* 1977). This method is also known as the Lanczos method in numerical analysis (Wilkinson 1964) and has been independently suggested as a way of finding the eigenvalues of a lattice Hamiltonian by Roomany *et al* (1980), who applied it to $Z(2)$ and $Z(3)$ Ising spin systems. Since this method has been described in some detail by Roomany *et al*, we content ourselves with a brief description and some comparisons of the two procedures.

The essential idea is to form a basis $|n\rangle$ in which H is tri-diagonal. Thus

$$H|n\rangle = b_n|n-1\rangle + a_n|n\rangle + b_{n+1}|n+1\rangle, \tag{2.13}$$

and the states $|n\rangle$ together with the coefficients $\{b_n, a_n\}$ can be calculated recursively from $b_0 = 0$ and an initial state $|0\rangle$ which we again choose to be the unperturbed eigenstate.

Considering the ground state of the 5-site Ising chain again, we take $|0\rangle = |.\rangle$ and hence

$$H|0\rangle = -x\sqrt{5}|\,|\,\rangle, \tag{2.14}$$

so that $a_0 = 0$, $b_1 = -x\sqrt{5}$ with

$$|1\rangle = |\,|\,|\rangle. \tag{2.15}$$

Repeating the operation gives

$$H|1\rangle = 4|1\rangle - x\sqrt{5}|0\rangle - 2x\sqrt{2}|2\rangle, \tag{2.16}$$

where

$$|2\rangle = \frac{1}{\sqrt{2}}(|\,|\,|\,|\,|\rangle + |\,|\cdot|\,|\rangle). \tag{2.17}$$

Yet another application of (2.13) forms the state

$$|3\rangle = \frac{1}{\sqrt{2}}(|\,|\,|\,|\,|\rangle - |\,|\cdot|\,|\rangle), \tag{2.18}$$

after which the recursion terminates leaving the tri-diagonal matrix representation

$$H = \begin{pmatrix} 0 & -x\sqrt{5} & 0 & 0 \\ -x\sqrt{5} & 4 & -2x\sqrt{2} & 0 \\ 0 & -2x\sqrt{2} & 6-3x & 2 \\ 0 & 0 & 2 & 2 \end{pmatrix}. \tag{2.19}$$

Since this matrix is tri-diagonal, the extraction of the lowest eigenvalue is easily achieved.

The termination of this recursion method is again due to the fact that the Ising Hamiltonian has a finite state space. For the O(2) model no such termination occurs, but successive estimates of the eigenvalues of H formed by truncating this recursion by putting $b_{N+1} = 0$ converge rather rapidly to the limiting value. This is illustrated in table 1, where we list successive estimates of the ground state energy of the 5-site chain for

Table 1. Successive estimates of the ground state energy and its derivative following from the recursion method for the 5-site O(2) Hamiltonian at coupling $x = 1$.

Order	$E_0(x)$	$E_0'(x)$
1	0	0
2	−0·870 83	−2·672 61
3	−1·128 26	−4·047 61
4	−1·240 72	−4·801 46
5	−1·273 91	−4·993 30
6	−1·285 32	−5·035 95
7	−1·288 16	−5·040 92
8	−1·288 91	−5·040 00
9	−1·289 14	−5·038 65

coupling $x = 1$. Evidently successive estimates are upper bounds to the exact level. This is indeed the case and can be established analytically (Wilkinson 1964). The procedure can be repeated for the first excited state by starting the recursion from the state $|0\rangle = |\,|\rangle$. The method may also be adapted to yield successive estimates of the derivative. Illustrative data for this are also presented in table 1.

The advantage of the recursion method is that it eliminates the necessity of explicitly diagonalising a large matrix. Thus the recursion method in principle can go further than the strong-coupling procedure. Nevertheless, it is still limited by the necessity of storing the states $|n\rangle$ in some appropriate basis, which is most easily taken to be the strong-coupling eigenstates of W_0. Thus the storage requirements of the two methods are comparable. Moreover, in practice one has to run the recursion method to higher order, thereby generating more states, to obtain results of sufficient accuracy. Indeed, we were unable to go beyond the limit of $M = 6$ achieved by the strong-coupling procedure without the necessity of an extensive use of external storage devices. If the storage problem can be overcome, the recursion method, because of its avoidance of any explicit diagonalisation, will probably be a significant step to tackling more complex Hamiltonians on higher-dimensional lattices. Unfortunately, this is a problem for which we do not see an early solution.

3. Mass gap of O(2) Hamiltonian

Figure 2 shows the estimates of the O(2) model mass gap $F(x, M)$ as a function of lattice size M. They decrease rapidly as x increases, but never actually vanish, which, of course, reflects the absence of a phase transition for finite M.

The key questions now are whether we can infer from these finite-lattice results: (i) the existence of a phase transition in the limiting ($M \to \infty$) system; (ii) that the low-temperature (large-x) phase is massless, i.e. the mass gap is zero; and (iii) at the

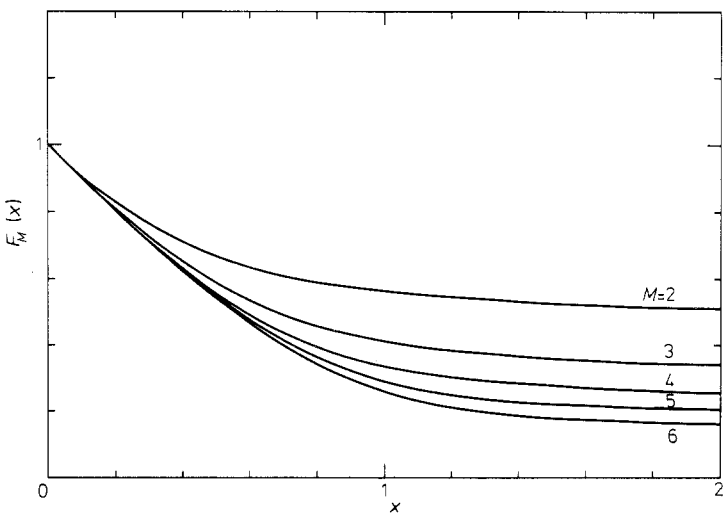

Figure 2. Mass gaps $F_M(x)$ for the O(2) Hamiltonian as a function of lattice size M.

onset of the massless phase, the mass gap vanishes exponentially as

$$F(x, M=\infty) \sim \exp\left[-a/(x-x_c)^{\sigma}\right] \tag{3.1}$$

where from Kosterlitz's (1974) analysis of the Euclidean action we expect $\sigma = \frac{1}{2}$.

To answer these questions we make use of finite-size scaling (Fisher and Barber 1972), which was described in some detail and extended to Hamiltonian field theory in I. The essential result for our present purpose is the *ansatz* that

$$F(x; M) \simeq M^{-1} Q(x/\xi) \tag{3.2}$$

where $\xi = 1/F(x; \infty)$ is the correlation length of the bulk system. Thus, if ξ is infinite,

$$F(x, M) \sim M^{-1}. \tag{3.3}$$

Elsewhere (Hamer and Barber 1980) we have argued that scale-invariant points in the infinite system can thus be identified by plotting

$$R_M(x) \equiv MF(x; M)/(M-1)F(x; M-1) \tag{3.4}$$

against x and finding those points for which

$$R_M(x) = 1. \tag{3.5}$$

For the Ising model (see I) the method yielded an estimate of $x_c = 1$ to less than 0·05% from data for $M \leqslant 10$. The method is equivalent to the prescription of 'phenomenological renormalisation' (Nightingale 1976, Sneddon and Stinchcombe 1979).

The ratios $R_M(x)$ for the O(2) model are plotted in figure 3. Their behaviour is remarkable. The ratios drop to within a fraction of one per cent of the value of 1 at $x \simeq 2$, and then stay there, being apparently asymptotic to the curve $x = 1$! This behaviour is established immediately, even for M as low as 3. We regard this as a spectacular demonstration that the O(2) model has a region of scale invariance in which it is massless. For comparison we note that, in a similar plot for the Ising Hamiltonian (see Hamer and Barber 1980), the ratios $R_M(x)$ for all M drop linearly through $x_c = 1$, thereby providing a clear indication of the presence of a single scale-invariant critical point. In the O(2) case it is hard to decide the precise position of the critical point with any accuracy when the ratios $R_M(x)$ are tangent to the line $x = 1$ at $x = x_c$, rather than crossing it. However, we estimate it to be at $x_c = 1{\cdot}8 \pm 0{\cdot}2$, which is in good agreement with the series analysis results of Hamer *et al* (1979).

To analyse the behaviour of the mass gap at the terminus of the massless region, it is convenient to investigate the β function defined (see Hamer *et al* 1979) by

$$\beta(g)/g = F(x)/[F(x) - 2xF'(x)]. \tag{3.6}$$

If $F(x)$ varies as in (3.1), then

$$\beta(g)/g \sim (x-x_c)^{1+\sigma}, \qquad x \to x_c, \tag{3.7}$$

i.e. the β-function vanishes algebraically, rather than with a simple zero as for a conventional transition.

Since the mass gap at criticality scales as

$$F(x_c, M) \sim 1/M, \qquad M \to \infty, \tag{3.8}$$

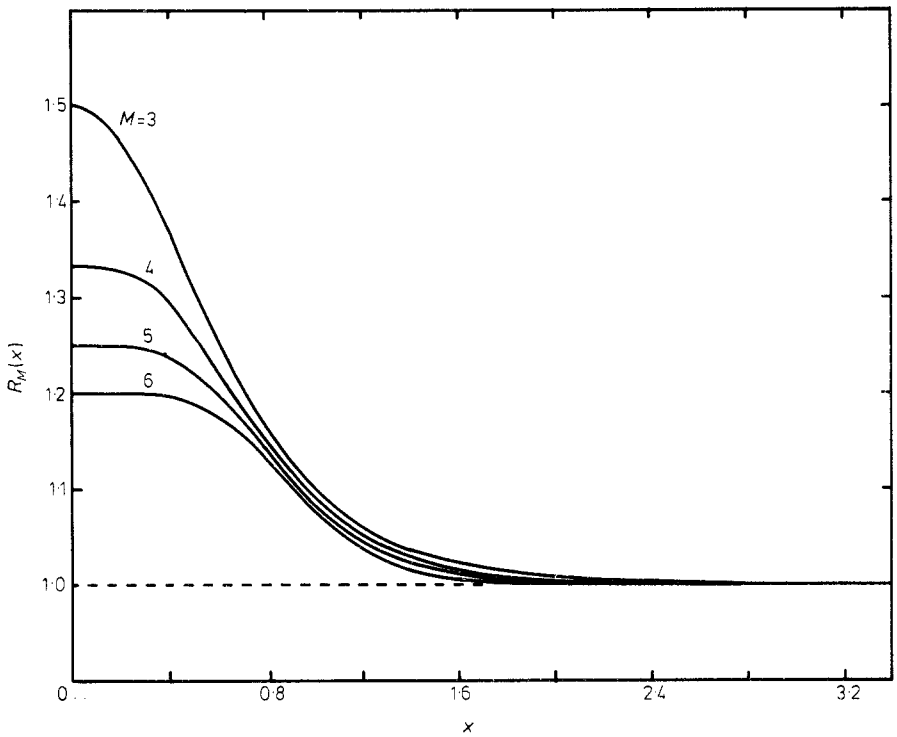

Figure 3. Scaled mass gap ratios $R_M(x) \equiv MF_M(x)/(M-1)F_{M-1}(x)$ against x for the O(2) model.

it is easy to show that the β function should vanish as

$$\beta(g)/g|_{x=x_c} \sim (\ln M)^{-(1+\sigma)/\sigma}, \qquad M \to \infty \tag{3.9}$$

as the lattice size increases†.

The finite-lattice results for the O(2) model β function are shown in figure 4. Unfortunately, values at $x_c \simeq 1{\cdot}8$ do not obey the scaling relation (3.9) at all well. However, the minimum values for each M scale somewhat better‡. These minimum values are listed in table 2. From successive pairs of points in table 2, one can deduce a slope for the plot of $\ln(\beta/g)$ against $\ln(\ln M)$ and hence an estimate of $(1+\sigma)/\sigma$. These slopes are also listed in table 2, along with linear and quadratic extrapolants of the slope against $1/M$. Our final estimate derived from these values is

$$(1+\sigma)/\sigma = 2{\cdot}1 \pm 0{\cdot}5, \qquad \text{i.e. } \sigma = 0{\cdot}9 \pm 0{\cdot}4. \tag{3.10}$$

There is a strong upward drift in the estimates of $(1+\sigma)/\sigma$ as M increases, with a corresponding downward drift in the estimates for σ, so that the value of $\sigma = \frac{1}{2}$ predicted by Kosterlitz (1974) is by no means unlikely. This behaviour also accords well with the

† For a conventional continuous transition at which the mass gap vanishes algebraically, the analogous prediction (see I) is $\beta(g)/g|_{x=x_c} \sim M^{-1/\nu}$.

‡ This is not unusual in finite-size scaling analyses where the exact critical coupling is not known, e.g. specific heat maxima are often used to estimate specific heat exponents from Monte Carlo data (see Domany *et al* 1975).

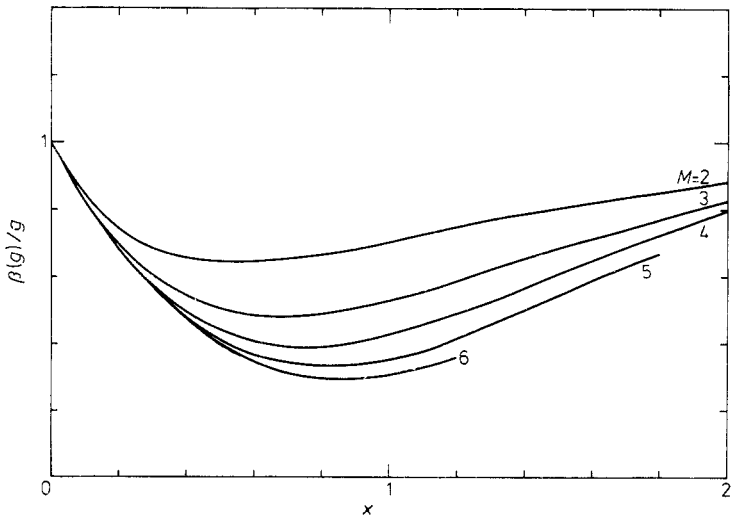

Figure 4. Values of the β function $\beta(g)/g$ of the O(2) model plotted as a function of $x = 2/g^2$ for various lattice sizes M. Note the definite minima.

Table 2. Minimum values of $\beta(g)/g$ for each lattice size M. From each successive pair of values, a slope can be deduced for the curve $\ln[\beta(g)/g]_{\min}$ against $\ln(\ln M)$. The estimates $l_M^{(1)}$ and $l_M^{(2)}$ are extrapolations of the slopes to $1/M = 0$ assuming (1) linear and (2) quadratic behaviour in the variable $1/M$.

M	$[\beta(g)/g]_{\min}$	Slope	$l_M^{(1)}$	$l_M^{(2)}$
2	0·642			
3	0·483	−0·62		
4	0·394	−0·88	−1·65	
5	0·337	−1·06	−1·78	−1·98
6	0·296	−1·20	−1·89	−2·09

more complicated form

$$F(x) \sim \exp[-b/(t + c\sqrt{t})], \qquad t = x - x_c \to 0, \tag{3.11}$$

which was suggested recently by Doniach and Huberman (1979).

The result (3.10) is certainly not spectacular, even if compared with the estimate from the series analysis of the strong-coupling expansions of $0{\cdot}6 \pm 0{\cdot}3$ (Hamer and Kogut 1979). In addition, the finite-lattice results for the β function minima can be extrapolated with a similar, if not better, accuracy by assuming a variation of the form $M^{-1/\nu}$ consistent with a conventional singularity. Thus our results are consistent with the expected behaviour, but data from longer chains or a more refined method of analysis are necessary to yield quantitative agreement.

Finally, results for the specific heat (or more precisely the second derivative $\omega_0''(x)$ of the ground state energy) on finite lattices are presented in figure 5. The curves seem to be converging rapidly towards an asymptotic form ($M \to \infty$) with a level plateau out to $x \simeq 0{\cdot}9$, followed by a smooth descent towards zero; there is no sign of any divergence at

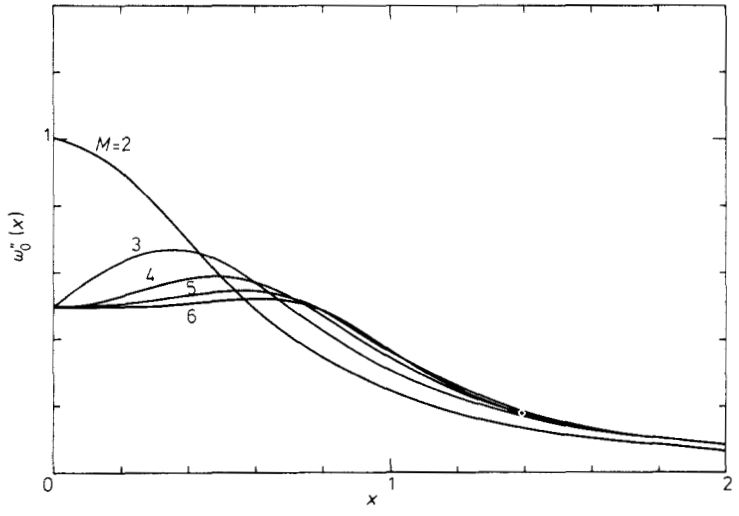

Figure 5. Plots of the second derivative of the ground state energy $\omega_0''(x)$ of the O(2) model against x for various lattice sizes M.

the critical point. This agrees with the series analysis (Hamer and Kogut 1979) and the renormalisation group arguments of Kosterlitz (1974).

4. The O(3) model

The mass gap $F(x, M)$ for the non-Abelian O(3) model is shown in figure 6. This model has more degrees of freedom than the O(2) model, of course; thus we have only been able to 'map' the function $F(x, M)$ reliably for 2- and 3-site lattices. The general

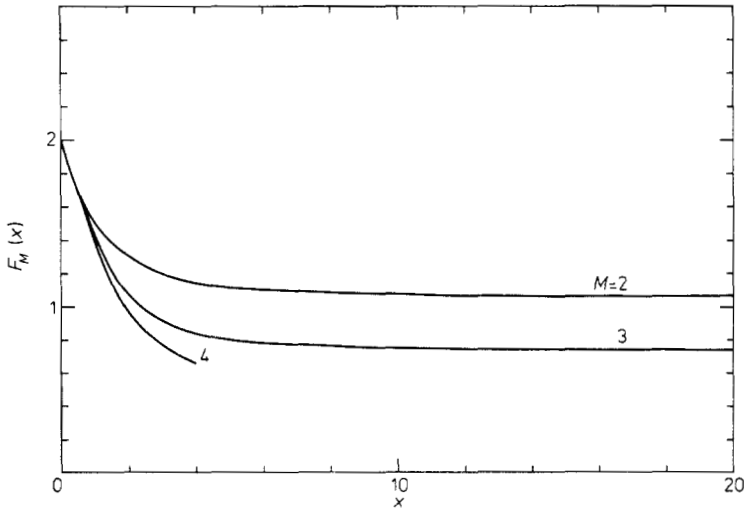

Figure 6. Mass gap values $F_M(x)$ for the O(3) model as a function of lattice size M.

pattern of behaviour appears very similar to that of the O(2) model. One might suspect the existence of a phase transition in the neighbourhood $x \simeq 10$.

The resulting values for the scaled mass gap ratio $R_M(x)$ are plotted in figure 7. The ratio for $M = 3$ drops rapidly, and then levels out, just as it did in the O(2) case. But it always remains safely above the critical value 1, by some 3 or 4%. We regard this as indicating the *absence* of a phase transition at finite x in the O(3) model.

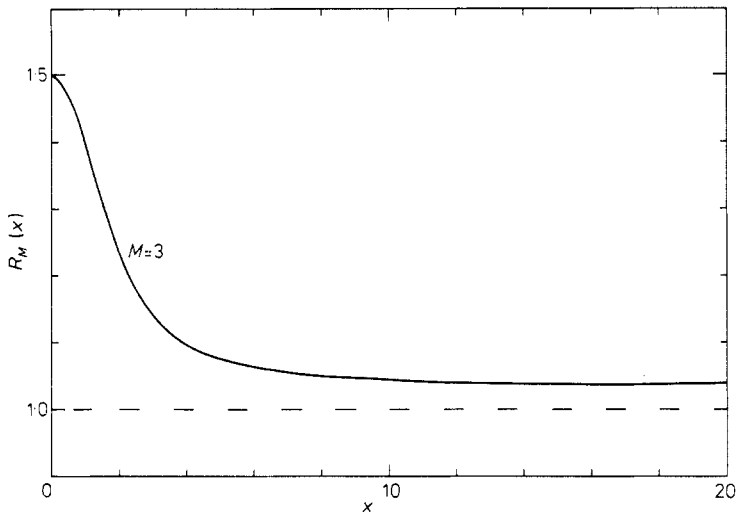

Figure 7. Plot of the scaled mass gap ratio $R_3(x)$ for the O(3) model.

This demonstration is not really conclusive, of course—we are stretching the finite-size scaling hypothesis to its very limits, and relying on it in a literal way for lattices down to the smallest size. We have no right in principle to do this. But the scaling hypothesis for the mass gaps has worked in such a sensitive and precise manner in the previous cases, that we are emboldened to rely on it here also.

By way of comparison, we recall that the strong-coupling series analysis for this model (Hamer and Kogut 1979) gave ambiguous results. The mass gap series in x did not seem to indicate a phase transition; but upon transforming to the variable $z = x/(1+x)$, the standard tests *did* indicate a phase transition at $x = 9 \pm 1 (z = 0{\cdot}9)$. It was only by matching the strong-coupling expansion with the weak-coupling results of Brézin and Zinn-Justin (1976) that one was able to reach a conclusion: namely that a phase transition was disfavoured (Hamer *et al* 1979, Hamer and Kogut 1979). This is in accord with theoretical prejudices, and with our finite-size scaling conclusion above.

We do not show curves for the specific heat (or rather $\omega_0''(x)$) in the O(3) model. The pattern is very similar to that of the O(2) model. There is a level plateau out to $x \simeq 2$, followed by a rapid, monotonic decline towards zero.

5. Analytic results for weak coupling

Our numerical results may be confirmed and illuminated by an algebraic analysis in the weak-coupling (low-temperature) limit, $x \to \infty$. We shall first consider the case of the

2-site lattice in some detail, and then indicate how these results may be extended to larger lattices.

Consider the dimensionless O(2) Hamiltonian

$$W \equiv \frac{2a}{g} H = \sum_{m=1}^{M} [J^2(m) - x \cos(\theta_m - \theta_{m+1})], \tag{5.1}$$

with periodic boundary conditions $\theta_{M+1} = \theta_1$, for the case $M = 2$. In an angular representation $J^2(m) \to -\partial^2/\partial\theta_m^2$, and if we change variables as follows,

$$\theta_+ = (\theta_1 + \theta_2)/\sqrt{2}, \qquad \theta_- = (\theta_1 - \theta_2)/\sqrt{2}, \tag{5.2}$$

then the eigenvalue equation for a 2-site lattice reads

$$-\left(\frac{\partial^2}{\partial\theta_+^2} + \frac{\partial^2}{\partial\theta_-^2} + 2x \cos(\sqrt{2}\,\theta_-)\right) u_l\{\theta\} = E_l u_l\{\theta\}. \tag{5.3}$$

This is Mathieu's equation. It cannot be solved in terms of simple functions, and the only analytic results available are power series expansions for small x and asymptotic expansions for large x. We shall now derive the leading terms in these two limits.

In the strong-coupling limit, $x \to 0$, the ground state and first excited state are simply eigenstates of the angular momentum operators:

$$u_0\{\theta\} = 1; \qquad \omega_0 = 0 \tag{5.4a}$$

$$u_1\{\theta\} = (\cos\theta_1 + \cos\theta_2) = 2\cos(\theta_+/\sqrt{2})\cos(\theta_-/\sqrt{2}); \qquad \omega_1 = 1. \tag{5.4b}$$

The limit $x \to \infty$ (weak coupling) is more interesting. The 'potential' term, $v(\theta_-) = -2x\cos(\sqrt{2}\,\theta_-)$, develops very deep wells, with periodic minima at the points

$$\theta_- = \sqrt{2}\,\pi m, \qquad m \text{ integer}. \tag{5.5}$$

The eigenfunctions have appreciable amplitudes only in the neighbourhood of these minima; in fact, to a first approximation they are delta functions, and for small θ_- we have

$$u_{0,1}\{\theta\} \simeq \delta(\theta_-), \tag{5.6a}$$

and hence

$$\omega_{0,1} \underset{x\to\infty}{\sim} -2x. \tag{5.6b}$$

To get a better approximation, one may consider 'small vibrations' near the well minima, approximating the wavefunction by a narrow Gaussian, so that the eigenvalues are found to be

$$\omega_{0,1} \underset{x\to\infty}{\sim} -2x + \sqrt{2x}. \tag{5.7}$$

These are the first two terms in an asymptotic series in powers of $1/\sqrt{x}$, which may be developed further by a more detailed analysis of the 'local' structure of the solutions near one of the well minima (e.g. Goldstein 1927).

Besides this local structure, however, the solutions also have a 'global', periodic structure, which gives rise to exponentially small corrections to the eigenvalues. The ground state, for instance, has period $\sqrt{2}\,\pi$ in θ_-, like the potential term; while the first excited state has period $2\sqrt{2}\,\pi$ in θ_- (cf equation (5.4*b*)). This structure is illustrated in figure 8.

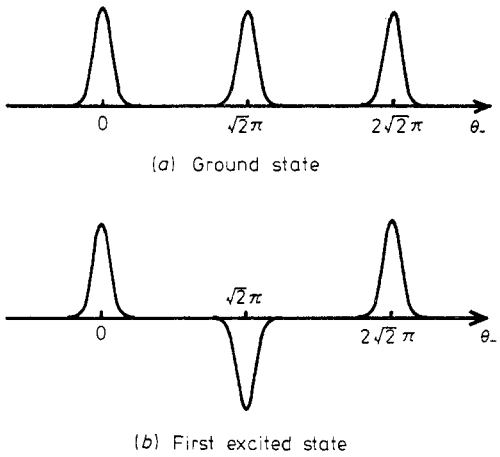

Figure 8. Structure of (*a*) the ground state and (*b*) the first excited state wavefunctions for the 2-site O(2) model.

The corrections to the eigenvalues arise in making connections between the solutions in the neighbourhood of adjacent minima. They are 'tunnelling' phenomena, arising as the wavefunction tunnels through the potential barrier between two minima. The magnitude of these effects may be estimated via the WKB approximation: they are proportional to

$$\exp\left\{-\int_0^{\sqrt{2}\pi} \mathrm{d}\theta_- \,[V(\theta_-)-E]^{1/2} \equiv \exp(-4\sqrt{2x})\right\}. \tag{5.8}$$

Now u_0 and u_1 are identical as regards their *local* structure in θ_-; they differ only in their global structure, as illustrated in figure 8, and in the fact that the 'average' angular momentum J_+^2 is 0 for u_0 and $\frac{1}{2}$ for u_1 (see equation (5.4)). Hence we find that the mass gap is

$$\omega_1-\omega_0 \underset{x\to\infty}{\sim} \tfrac{1}{2}+\mathrm{O}(\mathrm{e}^{-4\sqrt{2x}}). \tag{5.9}$$

This may be checked against the known solutions of Mathieu's equation (Goldstein 1929). It agrees with our numerical results, figure 2.

The basic features of the 2-site solution generalise quite easily to M sites. Again u_0 and u_1 have the same local structure in the vicinity of a potential well; they differ only in their global structure and in their 'average' angular momentum J_+^2, which is 0 for u_0 and $1/M$ for u_1. Hence the mass gap in the weak-coupling limit is

$$\omega_1-\omega_0 \underset{x\to\infty}{\sim} (1/M)+\mathrm{O}[\exp(-\mathrm{const}\sqrt{x})]. \tag{5.10}$$

The exponentially small correction term comes again from 'tunnelling' effects between one well minimum and its neighbour, i.e. from 'global' differences in the structure of u_0 and u_1.

We have thus shown analytically that in the limit $x\to\infty$ the mass gap scales exactly as $1/M$, behaviour characteristic of a critical point. If we neglected the exponential

'tunnelling' terms, this result would be true for *all* x, indicating a continuous line of critical behaviour and a massless phase, at all couplings. This conclusion, and the approximation from which it results, corresponds exactly to the spin wave approximation in conventional statistical mechanics (see e.g. Wegner 1967, José *et al* 1977).

The 'tunnelling' terms signal the presence of 'instantons' in the theory (Belavin *et al* 1975, 't Hooft 1976), which are the field theory analogues of the vortices considered by Kosterlitz and Thouless (1973) in statistical mechanics. According to the latter authors, they play a vital role in the phase structure of the theory. At low temperatures (large x) they are energetically disfavoured, and occur only in bound pairs of vortex and anti-vortex; this is the massless phase. At higher temperatures, however, their entropy of formation begins to have more effect, until eventually a phase transition occurs, and the vortices become unbound. Our numerical analysis bears out this picture.

For the O(3) model a similar analysis gives to leading order

$$\omega_1 - \omega_0 \underset{x\to\infty}{\sim} 2/M \tag{5.11}$$

for a lattice of M sites. We have not carried the analysis beyond leading order. Topological instantons do not exist for O(N), $N \geqslant 3$; but Belavin and Polyakov (1975) did discover pseudo-particle solutions of a different type for the O(3) case, and argued that they would destroy the massless phase at all couplings except $x = \infty$ (see also Trimper 1979). Whether this is the correct explanation is not clear, since the O(4) and higher models are expected to behave similarly to O(3), yet they have no instanton solutions. In any case, our numerical finite-lattice solutions do provide (weak) support for the absence of a phase transition at finite x.

6. Summary

In this paper we have extended our finite-lattice approach to Hamiltonian field theories to consider the behaviour of the O(2) and O(3) Heisenberg models in $(1+1)$ dimensions. Two methods of efficiently determining the low-lying eigenvalues of such Hamiltonians were described.

Finite-size scaling was used to formulate a remarkably sensitive test for a phase transition in the infinite system. The test involves the scaled mass gap ratio

$$R(x, M) = MF(x, m)/(M-1)F(x, M-1), \tag{6.1}$$

where M is the lattice size. According to finite-size scaling

$$R(x_c, M) \sim 1 \qquad \text{as } M \to \infty \tag{6.2}$$

at any point x_c for which the infinite system is scale-invariant, i.e. at which the correlation length of the infinite system diverges.

In practice, we have found that $R(x, M)$ satisfies (6.2) even for very small lattices, $M \geqslant 3$. For the Ising model (Hamer and Barber 1980, 1981), $R(x, M)$ dropped linearly through unity at $x \simeq x_c = 1$, indicating an isolated scale-invariant point. In the present work, plots of $R(x, M)$ for the O(2) model ($3 \leqslant M \leqslant 6$) approached unity and then stayed there for $x > x_c \simeq 1{\cdot}8$. We interpret this as strong evidence for the expected scale-invariant region at weak coupling (low temperatures). Finally, for the O(3)

model, $R(x, M)$ stays *above* unity for all finite x, leading us to conclude (albeit on the basis of a single curve, $M = 3$) that no phase transition occurs†.

We have also studied the weak-coupling limit of the O(2) model algebraically, and shown analytically that the mass gap scales like $1/M$ in the limit. Exponentially small correction terms were also found, corresponding to tunnelling phenomena or 'instantons'. These are the field theory analogues of the vortices discussed by Kosterlitz and Thouless (1973), which control the phase structure of the model. Thus all the essential physical features of the system (except, of course, the phase transition itself, which is a bulk phenomenon) are already present on the 2-site lattice. Even the smallest finite-lattice system provides a fascinating microcosm of the field theory.

The results reported here, together with those of I for the $(1+1)$-dimensional Ising Hamiltonian, and similar calculations by Roomany *et al* (1980) for $Z(2)$ and $Z(3)$ systems, suggest that finite-lattice methods are a viable procedure for investigating the phase structure of Hamiltonian field theories. Unlike perturbation expansions (Hamer *et al* 1979), they are capable of probing the whole of the phase diagram. Whether such methods can be brought to bear on more complex Hamiltonians, such as lattice gauge theories defined on higher-dimensional lattices, depends on the solution of some major computer problems. These are certainly difficult, but hopefully not insurmountable.

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† Note added. Since this work was done, Roomany and Wyld have improved upon our computer methods, and extended the results for the O(3) model to $M = 5$. Their conclusion is the same as ours (Roomany and Wyld 1980).

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