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LETTER TO THE EDITOR

Finite-size scaling in Hamiltonian field theory

C J Hamer† and Michael N Barber‡§

† Department of Theoretical Physics, Research School of Physical Sciences, Australian National University, Canberra, PO Box 4, ACT 2600, Australia

‡ Department of Physics, University of Washington, Seattle, WA 98195, USA

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Abstract. A new method for investigating the behaviour of lattice Hamiltonian field theories is described. The method uses finite-size scaling to extrapolate finite-lattice results to the infinite chain limit. The technique is illustrated by application to the transverse Ising model and the O(N)-Heisenberg Hamiltonians ($N = 2, 3$) in $(1+1)$ dimensions. The accuracy of the method appears comparable to or better than existing approaches.

Hamiltonian field theories on spatial lattices are of interest both in statistical mechanics and field theory (for a review see Kogut 1979). Currently, the only reliable method of investigating the critical behaviour and phase diagrams of such theories is through the analysis of the Rayleigh–Schrödinger perturbation series (see e.g. Hamer *et al* 1978, 1979). Attempts have been made to use renormalisation group techniques (Drell *et al* 1976, Jullien *et al* 1978) but as yet such methods do not offer comparable numerical accuracy even for simple systems.

In this Letter, we propose a new method which uses finite-size scaling (Fisher and Barber 1972) to extract the behaviour of the infinite lattice theory from the way physical quantities of interest vary with lattice size. In particular, we illustrate these ideas by summarising a series of finite-lattice calculations of the mass gap and β-function for the Hamiltonian versions of the two-dimensional Ising and O(N)-Heisenberg ($N = 2, 3$) models. Our results indicate that this procedure has an accuracy comparable to or better than that of series methods. Full details and further applications will be reported elsewhere.

We begin with the Ising model. The relevant quantum Hamiltonian (Fradkin and Susskind 1978) is

$$H = (g/2a) \sum_{m=1}^{M} \{1 - \sigma_3(m) - x\sigma_1(m)\sigma_1(m+1)\}. \qquad (1)$$

Here $\sigma_1(m)$ are Pauli matrices, g is a dimensionless coupling constant (proportional to temperature), a is the lattice spacing, $x = 2/g^2$ and the sum is over the M sites of a chain with periodic boundary conditions. In the limit $M \to \infty$, the ground state energy and mass gap of this model are known exactly (Pfeuty 1970). We have investigated the behaviour for finite M both analytically and numerically. Here we focus attention on

§ Permanent address: Department of Applied Mathematics, University of New South Wales, PO Box 1, Kensington, NSW2033, Australia.

the mass gap

$$F(x, M) = (2a/g)(E_1 - E_0), \tag{2}$$

where E_0 and E_1 are the energies of the ground state and first excited state respectively.

The mass gap of (1) for finite M can be determined analytically using standard fermion techniques (see e.g. Schultz *et al* 1964). Analysis of this result leads to the following conclusions.

(i) For fixed $x \neq 1$, $F(x, M)$ approaches its known limiting value exponentially fast in M; ie

$$F(x, M) = 2|1-x| + O(e^{-|1-x|M}), \qquad M \to \infty. \tag{3}$$

(ii) On the other hand, at $x = x_c = 1$,

$$F(1, M) = \pi/4M + O(M^{-3}). \tag{4}$$

(iii) Finally, if we consider a *uniform* limit, $x \to 1$, $M \to \infty$ with $(1-x)M = O(1)$, then

$$F(x, M) \approx M^{-1}O(|1-x|M), \tag{5}$$

where the scaling function can be computed exactly, and leads back to (3) and (4) in the appropriate limits.

These results are rather familiar. They are precisely the predictions which follow by extending the results of finite-size scaling from conventional statistical mechanics (Lagrangian field theory) to Hamiltonian field theory.

Let us recall the salient features of this theory (Fisher and Barber 1972). Let $\Psi(g)$ be some quantity which in an infinite system varies near some critical coupling g_c as

$$\Psi(g) = A|\Delta g|^{-\psi}, \qquad \Delta g = g - g_c \to 0. \tag{6}$$

Then in a finite system of *linear* dimension n, finite-size scaling asserts that the behaviour of $\Psi(g; n)$ is described by the ansatz:

$$\Psi(g; n) \approx n^{\psi/\nu} Q_\Psi(n/\xi(g)), \qquad n \to \infty, \Delta g \to 0. \tag{7}$$

Here $\xi(g)$ is the correlation length in the finite system, which diverges at g_c as

$$\xi(g) \simeq \xi_0|\Delta g|^{-\nu}. \tag{8}$$

Thus if g_c is known, (7) immediately implies that

$$\Psi(g_c; n) \simeq \text{const.}\ n^{\psi/\nu}, \qquad n \to \infty, \tag{9}$$

where for a logarithmic singularity ($\psi = 0$) the result is modified to

$$\Psi(g_c; n) \simeq \text{const.} \ln n, \qquad n \to \infty. \tag{10}$$

To apply these results to Hamiltonian field theory we simply make use of the standard relationships between statistical mechanics and field theory (Kogut 1979), in particular, that between the mass gap and the reciprocal of the correlation length. Hence if we identify Ψ in (7) and (9) with $1/\xi = F$, we immediately recover the exact results (4) and (5) provided $\nu = 1$, which is true (Pfeuty 1970). Alternatively, ν can be estimated directly for the behaviour of the β-function defined (Hamer *et al* 1979) by

$$\beta(g)/g = (d/dg) \ln[(g/2a)F(x)]. \tag{11}$$

In the infinite system this possesses a simple zero at x_c, while in the finite system, finite-size scaling predicts that

$$\beta(g_c, M) \approx M^{-1/\nu}, \qquad M \to \infty, \tag{12}$$

a result which can be confirmed analytically for the Ising Hamiltonian.

To test the predictive capabilities of finite-size scaling in the present context, we show in figure 1 a log–log plot of both the mass gap and the β-function evaluated at $x = x_c = 1$ for several values of M.

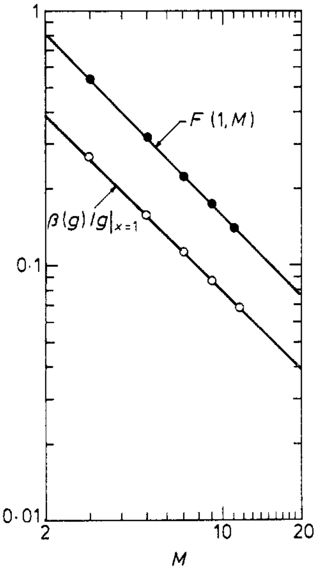

Figure 1. Log–log plots of finite lattice mass gaps (full circles) and β-functions (open circles) evaluated at $x = x_c = 1$ versus M. Straight lines have been drawn through each set of results.

The straight lines indicate that the scaling behaviour is established remarkably quickly. Equation (4) for the mass gap is confirmed to less than one percent, while from the β-function we estimate ν to be unity to a similar precision.

In practice, the critical value x_c of the coupling in the infinite system is often not known. The finite-size scaling form (4) suggests that g_c (or x_c) can be estimated from the sequence of values of x for which successive ratios of $F(x, M)$ and $F(x, M+1)$ exactly scale, i.e. the value of x for which

$$R_M(x) \equiv MF(x, M)/(M-1)F(x, M-1) = 1. \tag{13}$$

In figure 2, we exhibit a plot of $R_M(x)$ against x for various values of M. All curves drop quite rapidly through the value unity near $x = 1$ even for small M. This criterion is actually equivalent to that which follows by extending (Sneddon and Stinchcombe 1979) 'phenomenological renormalisation theory' (Nightingale 1976) to Hamiltonian field theory. It has been used previously to analyse numerical results for the mass gap of (1) (Sneddon and Stinchcombe 1979). As we shall now discuss, the criterion (13) also appears to be a very sensitive probe in more complex systems such as the O(N)-Heisenberg models.

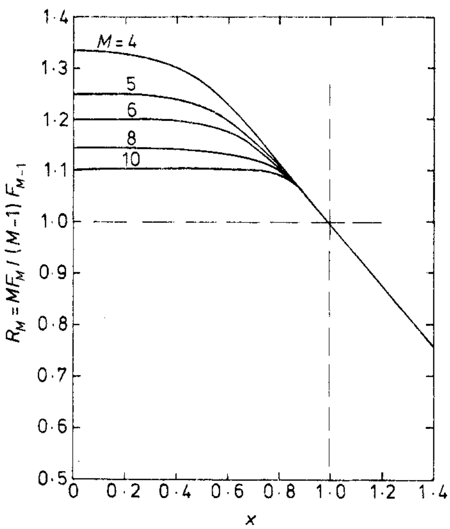

Figure 2. Plot of scaled mass gap ratios $R_M(x)$ versus x for the Ising model.

The lattice Hamiltonian version of these models takes the form (see e.g. Hamer *et al* 1979)

$$H = (g/2a) \sum_{m=1}^{M} \{\boldsymbol{J}^2(m) - x\boldsymbol{n}(m) \cdot \boldsymbol{n}(m+1)\} \tag{14}$$

where the notation is as before, except that $\boldsymbol{J}(m)$ is the angular momentum operator appropriate to $O(N)$ rotational symmetry and $\boldsymbol{n}(m)$ is an N-component spin vector normalised to unity. Strong coupling series for the mass gap and β-function of these models for $N \leqslant 4$ and $M = \infty$ have been derived and analysed by Hamer *et al* (1978, 1979) and Hamer and Kogut (1979).

Unfortunately, for finite M, it does not seem possible to derive any exact results and one must resort to a numerical procedure. However, unlike the Ising Hamiltonian, (14) has an *infinite* state space even on a finite chain. Thus no numerical procedure can presumably compute exact eigenvalues, and rather we require procedures which are sufficiently rapidly convergent to allow reasonably long chains to be investigated. We have devised two methods with this property.

The first is based on the same approach as used in the strong coupling expansions (Hamer *et al* 1979, Hamer 1979). Decompose (14) as $H = (g/2a)(W_0 - xV)$ where W_0 contains the single-site terms and V the coupling between sites. A set of strong coupling eigenstates of W_0 is now generated by successive applications of the operator V to an unperturbed eigenstate of W_0. Using this basis a finite matrix representation of H is calculated and its eigenvalues determined by standard methods. For a model such as the Ising model (1) with a *finite* state space, this method ultimately terminates yielding the exact eigenenergies of the finite chain. For the $O(N)$-models, sufficiently accurate results follow by perturbing to sufficiently high order ($\sim O(M)$). Most of our results have been obtained by this procedure.

We have also explored to some extent an alternative scheme in which H is reduced to a tri-diagonal form. Eigenenergies and other physical quantities can then be obtained iteratively without any explicit diagonalisation. The method is similar to recursive techniques used extensively in band theory (see e.g. Haydock *et al* 1975) and nuclear physics (see e.g. Whitehead *et al* 1977). In the context of Hamiltonian field theory it appears to have a slight storage advantage over the first method and may allow larger chains to be investigated. This approach has in fact been applied to $Z(2)$ and $Z(3)$-Ising spin systems by Roomany *et al* (1979).

Using these methods we have been able to calculate the energies of the ground state and first excited state for the O(2)-model up to $M=6$. The ratios $R_M(x)$ of successive mass gaps are plotted in figure 3. Their behaviour is remarkable. They drop to within a fraction of one percent of the value 1 at $x \simeq 2$ and then *stay* there. This behaviour is established immediately even for M as low as 3. We regard this as a spectacular demonstration of a region of scale invariance. Such a region is of course expected (Kosterlitz 1974, José *et al* 1977). It is hard to decide the exact value at which the region commences, but we estimate it to be at $x_c = 1{\cdot}8 \pm 0{\cdot}1$. This value is in good agreement with the series analysis result of Hamer and Kogut (1979).

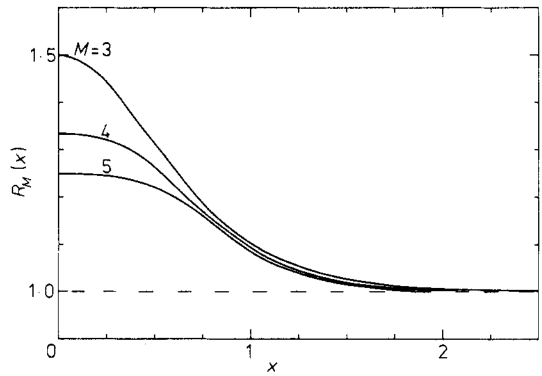

Figure 3. Plot of scaled mass gap ratios $R_M(x)$ versus x for the O(2)-model.

At x_c, one expects (Kosterlitz 1974) that in the infinite system the mass gap varies as

$$F(x) \sim \exp[-a/(x_c - x)^\sigma] \tag{15}$$

with $\sigma = \frac{1}{2}$. It then follows that the β-function has an *algebraic* singularity at x_c. The form (15) is not that usually adopted (see (8)) in the derivation of finite-size scaling results. However, it is easy to adapt the finite-size scaling analysis to incorporate this behaviour. The key prediction for our present purposes is that

$$\beta(g; M)/g|_{x=x_c} \sim (\ln M)^{-(1+\sigma)/\sigma}, \qquad M \to \infty. \tag{16}$$

Unfortunately, the value of β at $x_c \simeq 1{\cdot}8$ does not obey this relation very well. However, the *minimum* values of the β-function for each M do scale somewhat better and yield an estimate of $\sigma = 0{\cdot}9 \pm 0{\cdot}4$. While the accuracy of this value is not very impressive, it should be compared with the value of $\sigma = 0{\cdot}6 \pm 0{\cdot}3$ obtained by Hamer and Kogut (1979) via series analysis methods. Clearly results for larger lattices and a more refined method of analysis would be useful in this context. Nevertheless, it remains gratifying that the finite size analysis does give a clear indication (figure 3) of the scale invariant region.

We have finally applied the same method to the O(3)-Hamiltonian. This model has more degrees of freedom than the O(2)-model. Thus we have only been able to compute the mass gap reliably for two- and three-site lattices. The ratio $R_3(x)$ of these results remains distinctly above unity for all x, as one would expect if no transition occurs. While it is obviously unwise to place too much credence on this one calculation, it is significant that the corresponding quantities for the Ising and O(2)-models already exhibit the behaviour confirmed by results from larger chains. We hope to be able to extend the O(3)-results similarly.

In summary, we have described a method of investigating the behaviour of lattice Hamiltonians by scaling finite-lattice quantities to the infinite lattice limit. Extremely accurate results were thus obtained for the Ising model. Undoubtedly, this high accuracy reflects the simplicity of this model. Indeed, the accuracy for the O(2) and O(3) models was much poorer, but the expected behaviour was detected. Thus the method does seem to be a very sensitive qualitative indicator for the presence (or otherwise) of a phase transition, and its nature. We feel that this type of analysis should be useful in the investigation of more complex systems.

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