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Finite-lattice methods in quantum Hamiltonian field theory: I. The Ising model

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Abstract. A finite-size scaling formalism is outlined for quantum Hamiltonian field theory on a lattice. The scaling behaviour in the neighbourhood of a critical point is predicted. To test the theory, exact results are generated for the mass gap, specific heat and susceptibility of the $(1+1)$-dimensional Ising model on a finite lattice. Finite-size scaling methods give results for the critical parameters which are comparable in accuracy with those obtained by standard perturbation series analysis methods.

1. Introduction

The Hamiltonian field theory analogue of the two-dimensional Ising model was presented by Fradkin and Susskind (1978). This theory corresponds to an infinite one-dimensional Ising chain in a transverse field and exhibits a phase transition, the exact nature of which is known from the analytic solution of Pfeuty (1970). Thus this model provides a nice testing ground for approximate methods of investigating the behaviour of lattice Hamiltonians. Strong-coupling perturbation expansions have been calculated by Hamer *et al* (1978, 1979) for the mass gap, specific heat and susceptibility. From these expansions, critical parameters were then estimated by conventional ratio and Padé approximant methods. These estimates agreed particularly well with the expected behaviour. Various attempts (Drell *et al* 1976, Jullien *et al* 1978, Friedman 1976, Subbarao 1976) at renormalisation group calculations have also been made. However, as yet these methods do not have an accuracy comparable with that of the series methods.

In a recent Letter (Hamer and Barber 1980) we suggested the use of finite-size scaling (Fisher and Barber 1972b) to extrapolate finite-lattice quantities to the infinite-chain limit. In particular, we reported results for the (transverse) Ising model and the Hamiltonian version of two-dimensional O(N)-Heisenberg systems ($N=2, 3$) which suggested that this method could rival the series approach. The purpose of this paper is to give a detailed analysis of the behaviour of the transverse Ising model on a finite chain. Our aim is twofold; to establish analytically the validity of finite-size scaling, and then to discuss in detail the extraction of critical parameters using finite-size scaling from relatively small chains.

The paper is arranged as follows. In the next section, we briefly review finite-size scaling and extend it to Hamiltonian field theory. In § 3 we diagonalise the transverse

Ising model Hamiltonian on a finite chain and evaluate the ground state energy and mass gap. The latter quantity is explicitly shown to satisfy finite-size scaling in § 4, where we also calculate the appropriate scaling function. In § 5 we discuss to what extent we can extract the limiting behaviour from results computed on relatively small chains. Section 6 closes the paper with an overall summary and discussion, in which we compare the accuracy of this approach to other approximations.

2. Finite-size scaling

Finite-size scaling was originally developed in statistical mechanics by Fisher and Barber (1972b) to describe the effects of finite sample size on thermodynamic singularities occurring at critical points (see also Fisher 1971, 1973).

Let $\Psi(g)$ be some quantity (e.g. specific heat) which in an infinite system diverges at a critical value (g_c) of the coupling parameter g as

$$\Psi(g) \approx A|\Delta g|^{-\psi} \qquad \text{as } \Delta g = g - g_c \to 0. \tag{2.1}$$

Finite-size scaling then asserts that in a finite system of linear dimensions $L = na_0$, where a_0 is the lattice spacing, the behaviour of $\Psi(g; n)$ is described by

$$\Psi(g; n) \approx n^{\psi/\nu} Q_\Psi[n/\xi(g)]. \tag{2.2}$$

Here $\xi(g)$ is the correlation length of the infinite system which diverges as

$$\xi(g) \sim \xi_0|\Delta g|^{-\nu}, \qquad \Delta g \to 0. \tag{2.3}$$

The *ansatz* (2.2) is expected to be valid uniformly† in the limits $n \to \infty$, $g \to g_c$. To recover the behaviour (2.1) in the limit $n \to \infty$ at fixed (small) Δg we require

$$Q_\Psi(z) \approx A\xi_0^{-\psi/\nu} z^{-\psi/\nu} \qquad \text{as } z \to \infty. \tag{2.4}$$

In the event of a logarithmic singularity ($\psi = 0$) as occurs, for example, in the specific heat of the two-dimensional Ising model, (2.2) must be modified (Fisher and Barber 1972b, Fisher 1971) to

$$\Psi(g; n) - \Psi(g_1; n) \approx Q_\Psi[n/\xi(g)] - Q_\Psi[n/\xi(g_1)], \tag{2.5}$$

where g_1 is some fixed non-critical reference coupling. The limiting behaviour (2.4) of the scaling function $Q_\Psi(z)$ is similarly replaced by

$$Q_\Psi(z) = -(A/\nu) \ln z, \qquad z \to \infty. \tag{2.6}$$

At g_c, (2.2) immediately predicts that

$$\Psi(g_c; n) \approx Q_\Psi(0) n^{\psi/\nu}, \qquad n \to \infty. \tag{2.7}$$

The analogous result for a logarithmic divergence

$$\Psi(g_c; n) \approx (A/\nu) \ln n + O(1), \qquad n \to \infty, \tag{2.8}$$

follows from (2.5). Note that in this case the amplitude is given in terms of 'bulk' quantities. If g_c is known, these results allow the exponents of the transition in the infinite system (or at least the ratio ψ/ν) to be estimated from data on finite systems. If

† There is a tacit assumption made at this point that $\Psi(g; n)$ can be well-defined, e.g. (2.2) would not be valid for the spontaneous order which does not exist in a finite system.

g_c is not known, as would be more typical, (2.7) and (2.8) remain valid if $\Psi(g; n)$ is evaluated at some 'pseudo-critical' coupling $g_c(n)$ (e.g. the value of g for which $\Psi(g; n)$ is maximum), which approaches g_c no slower than $n^{-1/\nu}$ as $n \to \infty$.

These detailed predictions and indeed the basic *ansatz* (2.2) have been confirmed, often analytically, for many of the conventional models of statistical mechanics (Ferdinand and Fisher 1969, Barber and Fisher 1973a, b, Barber 1973, Ritchie and Fisher 1973, Capehart and Fisher 1976, Au-Yang and Fisher 1975). The utility of finite-size scaling in the analysis of Monte Carlo data has been illustrated by Domany *et al* (1975).

It is fairly straightforward to extend these concepts and results to Hamiltonian field theory. The essential result we require (see e.g. Kogut 1979, Scalapino *et al* 1972) is that the mass gap Λ_m (i.e. the energy difference between the first excited state and the ground state of the Hamiltonian theory) corresponds to the reciprocal of the correlation length $\xi(g)$. Thus for an infinite system exhibiting a conventional continuous transition $\Lambda_m(g)$ vanishes as

$$\Lambda_m(g) \sim |g - g_c|^\nu, \qquad g \to g_c. \tag{2.9}$$

Thus the behaviour of the mass gap in a finite system is described by the *ansatz*

$$\Lambda_m(g; n) \approx n^{-1} Q_\Lambda[n^{1/\nu}(g - g_c)], \qquad n \to \infty, \quad g \to g_c, \tag{2.10}$$

which follows by identifying Ψ in (2.2) with $1/\Lambda_m$. Note that, for future convenience, we have modified the argument of the scaling function. Equation (2.10) implies immediately that

$$\Lambda_m(g_c; n) \approx n^{-1} Q_\Lambda(0), \qquad n \to \infty, \tag{2.11}$$

a result we shall see is valid even for relatively small values of n.

Equation (2.10) also suggests that g_c could be estimated from the sequence of values of g for which successive ratios of $\Lambda_m(g; n)$ and $\Lambda_m(g; n+1)$ exactly scale, i.e. the value of g for which

$$n\Lambda_m(g; n) = (n+1)\Lambda_m(g; n+1). \tag{2.12}$$

This result is actually equivalent to the criterion for determining g_c that follows by extending 'phenomenological renormalisation theory' to Hamiltonian field theory (Sneddon and Stinchombe 1979). As originally formulated (Nightingale 1976), phenomenological renormalisation attempts to use finite-size results to derive an approximate recursion relation for the infinite system. Specifically, the correlation lengths $\xi(g; n)$ and $\xi(g; n')$ in two finite systems of 'sizes' n and n' are assumed to be related by

$$\xi(g; n) = b\xi(g'; n'), \tag{2.13}$$

with $b = n/n'$. In the limit that n and n' both become infinite with b fixed at some specific value, (2.13) represents the renormalisation of the correlation length under a renormalisation group transformation $g \to g' = R(g)$. For finite n and n', (2.13) is only approximate, but can be interpreted as defining an approximate mapping of the coupling constants from g to g'. The critical parameters now follow from the mapping in the standard way. This approach appears quite successful (Sneddon and Stinchcombe 1979, Nightingale 1976, 1977; Sneddon 1978, 1979).

One problem remains. The asymptotic result (2.7) yields the ratio ψ/ν. One would like to be able to determine ψ alone. Two posssibilities exist to do this. Firstly, if we invoke hyperscaling, ν is related to the specific heat index α by

$$d\nu = 2 - \alpha. \tag{2.14}$$

Thus the specific heat at g_c scales as

$$C(g_c; n) \sim n^{d\alpha/(2-\alpha)}. \tag{2.15}$$

(It should be noted that in applying (2.14) to a Hamiltonian theory, the dimensionality d must be taken to include the time dimension.) Alternatively, ν can be estimated directly from the observation that

$$[\partial \Lambda_m(g; n)/\partial g]_{g=g_c} \approx n^{-1+1/\nu} Q'(0) \tag{2.16}$$

which follows by differentiating (2.10); or equivalently,

$$\beta^{-1}(g_c; n) \equiv \frac{1}{\Lambda} \frac{\partial \Lambda}{\partial g}\bigg|_{g=g_c} \approx n^{1/\nu} \frac{Q'_\Lambda(0)}{Q_\Lambda(0)}, \tag{2.17}$$

where $\beta(g; n)$ is the Callan–Symanzik β function of the finite-lattice system (Hamer *et al* 1979). Equation (2.16) is also related to phenomenological renormalisation. According to the general renormalisation group theory (see e.g. Barber 1977), exponents follow from the recursion relations linearised about a particular fixed point. For a one-parameter recursion $g \to g' = R(g)$, ν is given by

$$b^{1/\nu} = (\mathrm{d}g'/\mathrm{d}g)_{g=g^*}, \tag{2.18}$$

where b is the spatial rescaling factor of the transformation and g^* the relevant fixed point. The derivative $\mathrm{d}g'/\mathrm{d}g$ can be estimated from (2.13), which gives

$$\left(\frac{\mathrm{d}g'}{\mathrm{d}g}\right)_{g=g^*} = \left(\frac{n'}{n}\right) \frac{\xi'(g^*; n)}{\xi'(g^*; n')}, \tag{2.19}$$

where $\xi' = \partial\xi/\partial g$. This result is thus simply an assertion that the finite-scaling prediction (2.16) is an *exact* scaling at g^*.

3. Transverse Ising model on a finite chain

The field theory version of the Ising model, in one space and one time dimension, has the simple Hamiltonian (Fradkin and Susskind 1978)

$$H = \frac{g}{2a} \sum_{m=1}^{M} [1 - \sigma_3(m) - x\sigma_1(m)\sigma_1(m+1)]. \tag{3.1}$$

Here the index m labels sites on a spatial lattice, while the time variable is taken to be continuous. The σ_i are Pauli matrices acting on a two-state spin variable at each site, g is a dimensionless coupling constant (proportional to temperature), a is the lattice spacing, M is the total number of sites and $x = 2/g^2$.

In the thermodynamic limit $M \to \infty$, this Hamiltonian has been diagonalised analytically by Pfeuty (1970). In particular, he found that the reduced mass gap

$$F(x) \equiv (2a/g)(E_1 - E_0), \tag{3.2}$$

where E_0 and E_1 are the energies of the ground state and first excited state of (3.1), was given by

$$F(x)=2|1-x|. \tag{3.2a}$$

Thus the model exhibits a phase transition at $x=1$ with the exponent $\nu=1$.

In this section we consider the behaviour of (3.1) on a finite chain of M sites with periodic boundary conditions. Using standard fermion techniques (Schultz *et al* 1964) we are able to evaluate the mass gap exactly. Our analysis, in fact, parallels that of Schultz *et al* (1964) for the transfer matrix of the two-dimensional (Lagrangian) Ising model very closely. This is not very surprising since (3.1) is obtained as the extreme anisotropic limit of the $d=2$ Ising transfer matrix (Fradkin and Susskind 1978). In view of this close relationship we omit all details of the diagonalisation of H.

It is convenient to define

$$W=\frac{2a}{g}H=M-\sum_{m=1}^{M}\sigma_3(m)-x\sum_{m=1}^{M}\sigma_1(m)\sigma_1(m+1), \tag{3.3}$$

where the periodic boundary conditions imply $\sigma_1(1)=\sigma_1(M+1)$. A transfer matrix of this form was considered by Schultz *et al* (1964). Using their methods, we find the following results for the two lowest eigenvalues of W.

The ground state energy is

$$\omega_0=M-\sum_{\substack{k=0\\(k\ \text{odd})}}^{2M-1}\Lambda\left(\frac{\pi k}{2M}\right), \tag{3.4}$$

and the first excited state energy is

$$\omega_1=M+2(1-x)-\sum_{\substack{k=0\\(k\ \text{even})}}^{2M-1}\Lambda\left(\frac{\pi k}{2M}\right), \tag{3.5}$$

where the function Λ is defined as

$$\Lambda(\theta)=[(1-x)^2+4x\sin^2\theta]^{1/2}. \tag{3.6}$$

Hence the mass gap can be written as

$$F(x,M)=\omega_1-\omega_0=2(1-x)+2M[T_{2M}(x)-T_M(x)], \tag{3.7}$$

where

$$T_N(x)=\frac{1}{N}\sum_{k=0}^{N-1}\Lambda\left(\frac{\pi k}{N}\right). \tag{3.8}$$

These results form the basis of our subsequent analysis.

Since for fixed x away from $x_c=1$, $\Lambda(\theta)$ is analytic in the strip

$$|\mathrm{Im}\,\theta|<\sinh^{-1}[(1-x)/2\sqrt{x}] \tag{3.9}$$

of the complex θ plane, we expect the sum $T_N(x)$ to converge to its formal limit

$$T_\infty(x)=\frac{1}{2\pi}\int_0^{2\pi}[(1-x)^2+4x\sin^2\theta]^{1/2}\,\mathrm{d}\theta \tag{3.10}$$

exponentially fast. This is confirmed in appendix 1, where we specifically establish that

$$F(x,M)-2(1-x)\sim\mathrm{O}(\exp\{-M\sinh^{-1}[(1-x)/2\sqrt{x}]\})\qquad \text{as } M\to\infty. \tag{3.11}$$

Right at $x = x_c = 1$, the mass gap is given explicitly by

$$F(1, M) = \sum_{k=0}^{2M-1} (-1)^{k-1} \sin\left(\frac{\pi k}{2M}\right), \tag{3.12}$$

which is readily evaluated to give

$$F(1, M) = 2 \tan(\pi/4M). \tag{3.13}$$

Hence as $M \to \infty$,

$$F(1, M) = \pi/2M + O(M^{-3}), \tag{3.14}$$

which immediately confirms the finite-size scaling prediction (2.11).

4. Finite-size scaling of mass gap

In the preceding section we saw that at $x = x_c = 1$, the mass gap of the transverse Ising model on a finite chain scales in accord with the predictions of finite-size scaling. Away from x_c, the approach to the infinite-chain limit was exponential in M. However, inspection of (3.11) shows that for $(1-x)$ of $O(M^{-1})$ this exponential approach will break down. This suggests introducing a *scaled* coupling

$$\mu = (1-x)M \tag{4.1}$$

and investigating the behaviour of the mass gap in the limit

$$M \to \infty, \qquad \mu = O(1). \tag{4.2}$$

This we do in this section and thereby explicitly confirm the basic finite-size scaling *ansatz* (2.10) for the mass gap.

From (3.4) and (3.5) we have, substituting (4.1) for x,

$$\begin{aligned} F(x, M) = 2\mu M^{-1} &- \sum_{\substack{k=0 \\ (k \text{ even})}}^{2M-1} \left[\frac{\mu^2}{M^2} + 4\left(1 - \frac{\mu}{M}\right) \sin^2\left(\frac{\pi k}{2M}\right)\right]^{1/2} \\ &+ \sum_{\substack{k=0 \\ (k \text{ odd})}}^{2M-1} \left[\frac{\mu^2}{M^2} + 4\left(1 - \frac{\mu}{M}\right) \sin^2\left(\frac{\pi k}{2M}\right)\right]^{1/2} \\ &= 2\mu M^{-1} + S_{2M}(2\mu) - 2S_M(\mu) + O(M^{-2}), \end{aligned} \tag{4.3}$$

where

$$S_N(\mu) = \sum_{k=0}^{N-1} \left[\frac{\mu^2}{N^2} + 4 \sin^2\left(\frac{\pi k}{N}\right)\right]^{1/2}. \tag{4.4}$$

For large N this sum can be analysed using the techniques of Barber and Fisher (1973a). This analysis is outlined in appendix 2, where we show that

$$S_N(\mu) = \frac{4N}{\pi} + \frac{2\mu^2}{\pi N}\left[\ln\left(\frac{2N}{\pi}\right) + C_E\right] - \frac{\pi}{N} R_{1\frac{1}{2},0}\left(\frac{\mu^2}{4\pi^2}\right) + \frac{\mu}{N} - \frac{\pi}{3N} + O(N^{-2}). \tag{4.5}$$

In this expression $C_E \approx 0{\cdot}572\ 134$ is Euler's constant and

$$R_{1\frac{1}{2},0}(z) = -4 \sum_{r=1}^{\infty} [(r^2 + z)^{1/2} - r - z/2r] \tag{4.6}$$

is a remnant function (Fisher and Barber 1972a). Substituting (4.5) in (4.3) yields the required expansion of the mass gap in the form

$$F(x, M) = M^{-1}Q(\mu) + \mathrm{O}(M^{-2}). \tag{4.7}$$

The scaling function is given explicitly by

$$Q(\mu) = \frac{\pi}{2} + \mu + \frac{4\mu^2}{\pi}\ln 2 - \frac{\pi}{2}R_{1\frac{1}{2},0}\left(\frac{\mu^2}{\pi^2}\right) + 2\pi R_{1\frac{1}{2},0}\left(\frac{\mu^2}{4\mu^2}\right). \tag{4.8}$$

Since by definition (4.1) μ is $(1-x)M$ and the exponent ν has value unity (Pfeuty 1970), (4.7) is precisely of the form (2.10) asserted by finite-size scaling.

Two limits of (4.8) are now of special interest: (i) $\mu \to 0$ corresponding to $x \to 1$ at fixed M; and (ii) $\mu \to \infty$ corresponding to $M \to \infty$ at fixed x (near μ). In the first limit we note that

$$R_{1\frac{1}{2},0}(z) = \mathrm{O}(z^2) \qquad \text{as } z \to 0 \tag{4.9}$$

and thus

$$Q(\mu) = \pi/2 + \mathrm{O}(\mu), \tag{4.10}$$

from which we immediately recover (3.14). In the opposite limit ($\mu \to \infty$) we require the asymptotic behaviour of the remnant function $R_{1\frac{1}{2},0}(z)$. This is given in appendix D of Barber and Fisher (1973a):

$$R_{1\frac{1}{2},0}(z) = z \ln z + 2z(c_{\mathrm{E}} - \ln 2 - \tfrac{1}{2}) + 2z^{1/2} - \tfrac{1}{3} + \text{const.} \times z^{1/2}\,\mathrm{e}^{-2\pi\sqrt{z}}. \tag{4.11}$$

Substituting this result in (4.8) yields

$$Q(\mu) = 2\mu + \mathrm{O}(\mathrm{e}^{-4\mu}) \tag{4.12}$$

and thus for $M \to \infty$ at fixed (small) $1-x$,

$$F(x, M) = 2(1-x) + \mathrm{O}(\mathrm{e}^{-M(1-x)/2}), \tag{4.13}$$

which reproduces (3.11).

5. Behaviour of short chains

In the preceding sections we have analytically established that finite-size scaling is exact for the mass gap of the transverse Ising model in the limit $M \to \infty$, $x \to 1$ with $(1-x)M$ of order unity. In this section we now want to consider the extrapolation of results derived for relatively short chains. To this end we have computed the mass gap, β function, specific heat and susceptibility for the Ising Hamiltonian (3.1) on a series of lattices of M sites with $M \leqslant 11$. The first three quantities can be numerically evaluated from the exact results (3.4) and (3.5). A similar closed expression for the susceptibility does not appear to be possible. However, exact numerical values can be computed by generating a finite-matrix representation of the Hamiltonian using strong-coupling eigenstates (Hamer and Barber 1980). Full details of this procedure are given in the following paper (Hamer and Barber 1981).

5.1. Mass gap and β function

Figure 1 shows the exact mass gaps as functions of x for various lattice sizes M. In the region $x < 1$, these curves evidently provide successively closer approximations to the

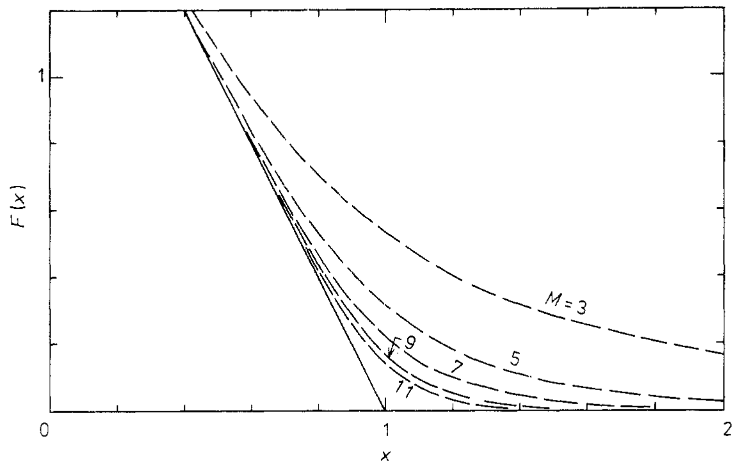

Figure 1. Mass gap $F(x)$ plotted against x. The broken curves are exact results for successively increasing lattice sizes and are labelled by the lattice size. The full curve is the exact result for the infinite lattice.

mass gap for the infinite system as M increases. In the neighbourhood of the critical point, however, the finite-lattice results swing away and tend asymptotically to the real axis from above. Thus the mass gap never vanishes on a finite lattice, in accord with the absence of any transition in an Ising model which is infinite in fewer than two dimensions.

To estimate the critical coupling we use (2.12) and compute x_s such that $R_M(x_s) = 1$, where $R_M(x)$ where

$$R_M(x) = \frac{M(x, M)}{(M-1)F(x, M-1)} \tag{5.1}$$

is the 'scaled mass gap ratio'. Successive estimates of x_s are tabulated in table 1, and evidently converge rather rapidly to $x_c = 1$. Empirically we find the convergence to be of order M^{-3}. Table 1 also lists values of $R_M(x)$ *at* $x_c = 1$. These also converge rapidly

Table 1. Finite-size behaviour of mass gap ratio.

Lattice size M	x_s ($R_M(x_s) = 1$)	$R_M(x_c = 1)$
3		0·97033
4	0·984127	0·98980
5	0·992680	0·99532
6	0·996032	0·99747
7	0·997610	0·99848
8	0·998450	0·99901
9	0·998938	0·99932
10	0·999241	0·99952
20	0·999913	0·99994
30	0·999975	0·99998
40		0·999993
50		0·999997

to unity. Equation (3.14) implies that this approach is *asymptotically* of $O(M^{-2})$, which is borne out by the numerical results even for rather short chains ($M \leq 10$). Thus finite-size scaling appears to work remarkably well. It should be noted that this rapid approach to the asymptotic limit is related to the absence of confluent correction terms in the Ising model, other than the integrally spaced powers expected from any Taylor expansion. For other systems, where a significant correction-to-scaling exponent is expected, the approach to the asymptotic finite-size scaling limits will be slower. Indeed, this is a conceivable way to extract the correction-to-scaling exponent.

The exponent ν may be estimated similarly, by using the β function

$$\frac{\beta(g)}{g} = \frac{F(x)}{F(x) - 2xF'(x)}. \tag{5.2}$$

Assuming the scaling behaviour (2.17), and the critical point $x_c = 1$, one can form estimates of the exponent ν from the finite-lattice results tabulated in table 2. It can be seen that the 10-site lattice gives ν correct to 0·5%; and extrapolation of the sequence of estimates using Padé or Shanks tables might be expected to procure a further order-of-magnitude increase in accuracy.

Table 2. Successive estimates of the exponent ν from the β function as a function of M.

Lattice size M	$B = \beta(g)/g$ $(x = 1)$	Estimate of $-1/\nu$, $S = [\ln B(M) - \ln B(M-1)]/[\ln M - \ln(M-1)]$
3	0·26795	−1·0743
4	0·19891	−1·0356
5	0·15838	−1·0210
6	0·13165	−1·0139
7	0·11267	−1·00990
8	0·09849	−1·00740
9	0·08749	−1·00574
10	0·07870	−1·00459
20	0·03929	−1·00108
30	0·02619	−1·00047
40	0·01964	−1·00026
50	0·01571	−1·00017

5.2. Specific heat

In statistical mechanics, the specific heat is the second derivative of the free energy with respect to temperature:

$$C = -T(\partial^2 G/\partial T^2). \tag{5.3}$$

Now the field theory analogue (Kogut 1979, Scalapino *et al* 1972) of the free energy is the ground state energy ω_0, and the analogue of temperature is the coupling g. Hence we can easily show that the strict analogue of the specific heat is

$$C = -(x/a)[\omega_0'(x) + 2x\omega_0''(x)], \tag{5.4}$$

where $x = 2/g^2$ as before. Now the divergence (if any) at the critical point will occur in ω_0'': and since we are not concerned here with any physical meaning, we shall define the 'specific heat' for the purposes of this paper to be

$$\tilde{C} = -x^2\omega_0''(x). \tag{5.5}$$

From Pfeuty's solution, the ground state energy per site for the infinite lattice is

$$\frac{\omega_0}{M} = 1 - \frac{2}{\pi}(1+x)E\left(\frac{\pi}{2}; m\right), \qquad m = \frac{4x}{(1+x)^2}, \tag{5.6}$$

where $E(\pi/2; m)$ is the complete elliptic integral of the second kind. Hence it follows that the specific heat per site is

$$\frac{\tilde{C}}{M} = \frac{8x^2}{\pi(1+x)^3}\left[\frac{4(1-x)^2}{(1+x)^2}E''\left(\frac{\pi}{2}; m\right) - 2E'\left(\frac{\pi}{2}; m\right)\right]. \tag{5.7}$$

From the properties of the elliptic integral (see e.g. Abramowitz and Stegun 1972) one may show that C/M has a logarithmic singularity at the critical point $x = 1$, as one expects for the Ising model:

$$\frac{\tilde{C}(x)}{M} \sim \frac{1}{\pi}\ln\left(\frac{1}{|1-x|}\right), \qquad x \to 1. \tag{5.8}$$

Numerically the finite-lattice results (3.4) for the ground state energy ω_0 provide a sequence of lower bounds to the ground state energy per spin of the infinite chain, which converges rather rapidly. The analysis of appendix 1 establishes that for *large M* this approach is exponential. Again it appears that the behaviour is established even for small values of M. The corresponding estimates of the specific heat are shown in figure 2. As expected, these curves are similar to those computed for finite two-dimensional Ising models (Ferdinand and Fisher 1969, Au-Yang and Fisher 1975).

Now finite-size scaling predicts—recall (2.8)—that the finite-lattice estimates of the specific heat at $x = 1$ will increase logarithmically with M; and similarly for the peak values at each M. These hypotheses are tested in figure 3, where it can be seen that this

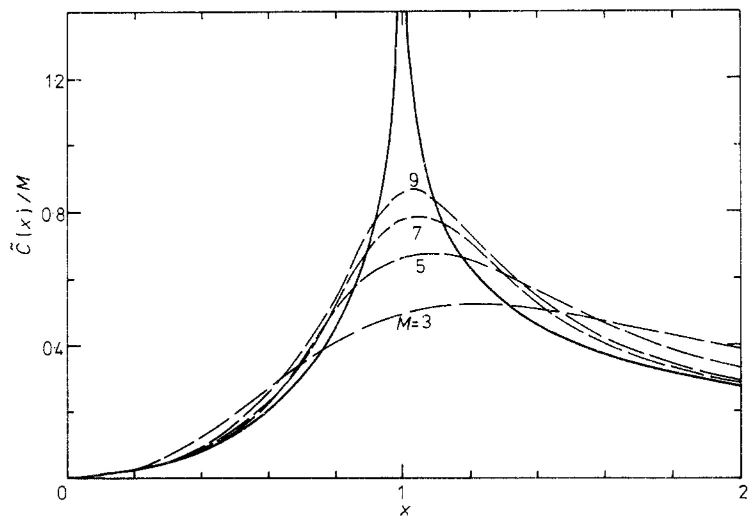

Figure 2. Finite-lattice results for the 'specific heat' $-x^2\omega_0''(x)$ as functions of x. The curves are labelled as in figure 1. The full curve is the result for an infinite lattice.

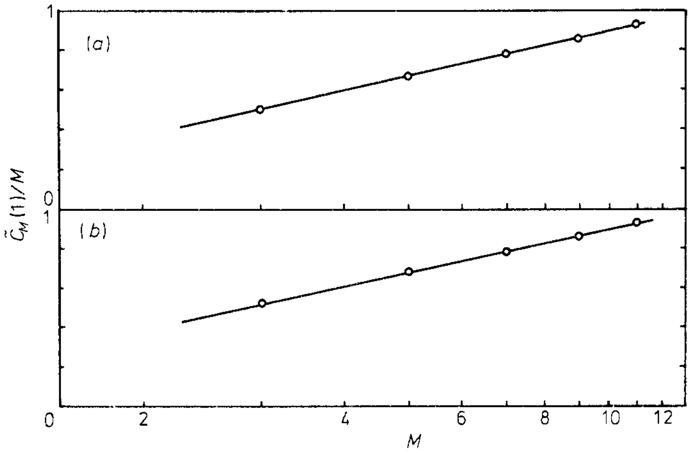

Figure 3. Semi-logarithmic plots of (*a*) specific heat estimates at $x = 1$ and (*b*) peak values of specific heat against M. Straight lines have been drawn through each set of results.

logarithmic behaviour is established immediately. Thus the scaling pattern again provides a good indication of the critical behaviour of the model. The slopes of the curves are 0·320, which agrees rather well with the theoretical prediction of A/ν, with $\nu = 1$ and $A = 1/\pi$ as given by (5.8).

5.3. *Susceptibility*

The Ising model Hamiltonian in the presence of an external magnetic field is

$$H = \frac{g}{2a} \sum_m [1 - \sigma_3(m) - x\sigma_1(m)\sigma_1(m+1) + h\sigma_1(m)], \tag{5.9}$$

where h is the magnetic field. In statistical mechanics, the magnetic susceptibility is defined by

$$\chi_T = -\left(\frac{\partial^2 G}{\partial h^2}\right)_T\bigg|_{h=0}. \tag{5.10}$$

The analogous quantity in field theory is therefore

$$\chi = -\left(\frac{\partial^2 \omega_0}{\partial h^2}\right)_x\bigg|_{h=0}. \tag{5.11}$$

An exact expression for this quantity has not been derived, to our knowledge; but an analysis of the strong-coupling series for χ has been carried out (Hamer *et al* 1978) giving a critical exponent $\gamma = 1{\cdot}76 \pm 0{\cdot}01$, which is equal within errors to the expected value of $\frac{7}{4}$.

The exact finite-lattice results for χ are shown in figure 4†. These curves show no peak as a function of x, so the only available scaling test concerns the values at the

† As noted earlier, these were computed numerically by a method described in the following paper (Hamer and Barber 1981).

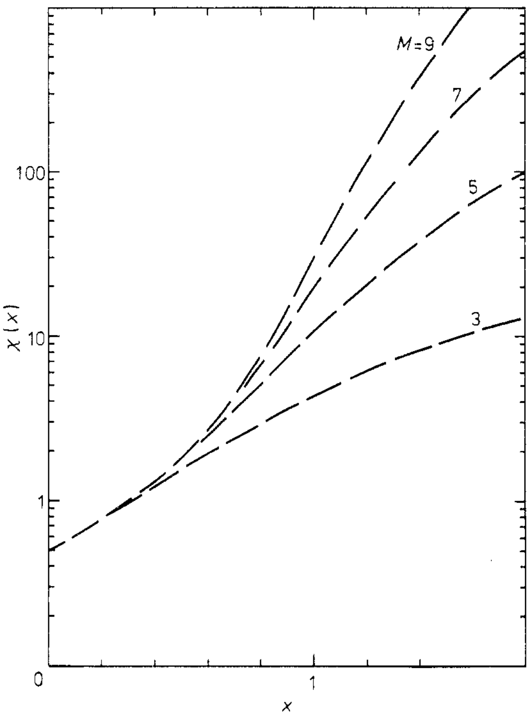

Figure 4. A semi-logarithmic plot of finite-lattice susceptibilities against x. Each curve is labelled by M as before.

critical point, $x = 1$. Finite-size scaling (equations (2.7)) predicts that

$$\chi_M(x=1) \sim M^{\gamma/\nu}, \qquad m \to \infty. \tag{5.12}$$

These values, together with the ratio $\log[\chi_M/\chi_{M-2}]/\log[M/M-2]$ for successive values of M, are shown in table 3. The latter numbers appear to be converging rather smoothly, and give an estimate $\gamma/\nu = 1{\cdot}750 \pm 0{\cdot}005$.

Thus the scaling of the finite-lattice results at the critical point can be used to estimate the critical index with an accuracy comparable with that of the perturbation series analysis method (Hamer and Kogut 1979). An advantage of this method appears to be the smooth convergence of the successive estimates, as compared with the series ratios which very often show oscillatory behaviour (Hamer and Kogut 1979).

Table 3. Successive estimates of the susceptibility critical index γ versus M.

M	$\chi_M(1)$	$\log[\chi_M(1)/\chi_{M-2}(1)]/\log[M/M-2]$
3	4·33	
5	10·78	1·786
7	19·51	1·763
9	30·35	1·758
⋮		
∞		1·750 ± 0·005 (extrapolated estimate)

6. Summary and conclusions

In this paper, we have studied the behaviour of the Hamiltonian field theory version of the Ising model on a finite lattice. In particular, we showed that finite-size scaling was exact for the mass gap of the theory, and finite-size scaling can be used to extract estimates of the critical parameters.

The mass gap, for example, is expected to vary inversely as the size of the lattice at the critical point: by searching for this behaviour, one can locate the critical point with excellent accuracy. The specific heat and susceptibility at the critical point are expected to scale with the size of the lattice like $M^{\alpha/\nu}$† and $M^{\gamma/\nu}$ respectively: by testing for this behaviour, one can estimate the critical exponents α/ν and γ/ν. Similarly the β function should behave as $M^{-1/\nu}$, which allows an independent determination of ν. It was discovered that this scaling behaviour was established very early (at low values of M) for this simple model.

We have found that these tests give results for the critical parameters which are comparable in accuracy with those obtained by standard perturbation series analysis methods (Hamer *et al* 1979, Hamer and Kogut 1979). Furthermore, the finite-lattice estimates provide a picture of the quantities involved over the whole range of couplings, which should be extremely useful in cases where the critical behaviour is unusual, or where there is no critical point at all. It has been argued elsewhere (Hamer 1979) that these approximations should be more accurate and reliable than those obtained by joining Padé approximants to the perturbation power series. Hence we expect the method to be an important adjunct and alternative to that of series analysis.

It is also useful to compare the accuracy of our determination of the critical properties of the one-dimensional transverse Ising model with that of recent renormalisation group calculations. These calculations all involve splitting the lattice into blocks which are diagonalised exactly. They differ in how the iteration is implemented. The simplest scheme (Drell *et al* 1976, Jullien *et al* 1978) is to completely neglect all block states except a few of the lowest energy. The most accurate calculation of this form (Jullien *et al* 1978) using a block of 7 sites gave (in our notation) $x_c = 1{\cdot}053$, $\nu = 1{\cdot}16$ and $\gamma = 1{\cdot}73$. Somewhat better accuracy for x_c and ν but not for the exponents β or γ is obtained if all states of a block are retained and effective Pauli spin operators introduced at each iteration (Friedman 1976, Subbarao 1976). The recursion relation, however, can now only be realised perturbatively in the coupling constants. To first order this yields (Subbarao 1976) $x_c = 1{\cdot}01$, $\nu = 1{\cdot}13$.

Like our approach, such renormalisation group calculations can also produce 'pictures' of physical quantities for all couplings. Unlike our pictures, these approximations are non-analytic. On the other hand, our results have the advantage of approaching the limiting infinite-system curves rather rapidly except in the immediate vicinity of the critical point. This is certainly not the case for a renormalisation group calculation as can be seen by comparing our figure 2 of the specific heat with figure 2 of Julien *et al* (1978) for the same quantity.

A renormalisation group calculation which is rather closer in spirit to our approach is that of Sneddon (1978) using phenomenological renormalisation. As discussed in § 3 phenomenological renormalisation is related to finite-size scaling; the key equation being equivalent to equation (2.12). The significant differences between Sneddon's

† This is the general result. In the special case of the two-dimensional Ising model we have $\alpha = 0$, and logarithmic behaviour occurs instead.

work and that reported here are the use (i) of exact finite-lattice eigenvalues and (ii) of finite-size scaling to extract other exponents.

The use of exact finite-lattice eigenvalues is, of course, special to this rather simple model. For more complex and interesting models, the finite-size eigenvalues have to be determined numerically (Hamer and Barber 1981) by some appropriate algorithm. In the following paper we describe two methods for doing this, and show that finite-size scaling remains a powerful and useful tool for investigating the behaviour of the limiting system.

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Appendix 1. Asymptotic behaviour of mass gap for fixed x

In this appendix we show that, for fixed x away from x_c, the mass gap $F(x, M)$ approaches its infinite-lattice limit exponentially fast in M. It is convenient to rewrite (3.20) for $F(x, M)$ as

$$F(x, M) = 2(1-x) + 2M\sqrt{x}[\tilde{T}_{2M}(x) - \tilde{T}_M(x)], \tag{A1.1}$$

where

$$\tilde{T}_M(x) = \frac{1}{M}\sum_{k=0}^{M-1} \tilde{\Lambda}\left(\frac{2\pi k}{M}\right) \tag{A1.2}$$

with

$$\tilde{\Lambda}(\theta) = (\lambda^2 + 2 - 2\cos\theta)^{1/2} \tag{A1.3}$$

and

$$\lambda^2 = (1-x)^2/x. \tag{A1.4}$$

For fixed non-zero λ, the sum $\tilde{T}_M(x)$ can be analysed using the Poisson summation formula (see e.g. Barber and Fisher 1973a).

Let

$$\tilde{\Lambda}(\theta) = \sum_{k=-\infty}^{\infty} c_k\, e^{ik\theta}, \tag{A1.5}$$

where

$$c_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ik\theta}\tilde{\Lambda}(\theta)\, d\theta. \tag{A1.6}$$

Hence substituting (A1.5) in (A1.2) we obtain

$$\tilde{T}_M(x) = c_0 + \sum_{l=1}^{\infty} (c_{lM} + c_{-lM}), \tag{A1.7}$$

where

$$c_0=\frac{1}{2\pi}\int_{-\pi}^{\pi}\tilde{\Lambda}(\theta)\,\mathrm{d}\theta \tag{A1.8}$$

is the limit of $\tilde{T}_M(x)$ as $M\to\infty$. To estimate the correction terms we therefore need the behaviour of c_k for large k. To analyse c_k we put

$$w=\tfrac{1}{2}\mathrm{i}\theta, \qquad w_c=\sinh^{-1}(\tfrac{1}{2}\lambda), \tag{A1.9}$$

so that

$$\tilde{\Lambda}(\theta)=2[\sinh(w_c+w)\sinh(w_c-w)]^{1/2}, \tag{A1.10}$$

and the contour of integration in (A1.6) now runs from $w=-\frac{1}{2}\pi\mathrm{i}$ to $\frac{1}{2}\pi\mathrm{i}$. Shifting the contour to run along Re $w=w_c$ yields

$$c_k=c_{-k}=\mathrm{e}^{-2|k|w_c}A_k(\lambda), \tag{A1.11}$$

where

$$A_k(\lambda)=\frac{2}{\pi\mathrm{i}}\int_{-\frac{1}{2}\pi\mathrm{i}}^{\frac{1}{2}\pi\mathrm{i}}\mathrm{e}^{-2|k|w'}[\sinh(-w')\sinh(w'+2w_c)]^{1/2}\,\mathrm{d}w. \tag{A1.12}$$

The singularity is now at $w'=0$ but is clearly integrable. Further deformation of the contour so that it runs along the two sides of the branch out from $w'=0$ to ∞ yields

$$A_k(\lambda)=2\int_0^{\infty}\mathrm{e}^{-2(k)s}p(s)\,\mathrm{d}s, \tag{A1.13}$$

with

$$p(s)=\frac{1}{\pi\mathrm{i}}\{[\sinh(s\,\mathrm{e}^{-\mathrm{i}\pi})\sinh(s+2w_c)]^{1/2}-[\sinh(s\mathrm{e}^{\mathrm{i}\pi})\sinh(s+2w_c)]^{1/2}\}$$
$$\approx 2s^{1/2}(\sinh 2w_c)^{1/2}+\mathrm{O}(s) \qquad \text{as } s\to 0. \tag{A1.14}$$

Since for large k the dominant contribution to the integral in (A1.13) comes from the behaviour of $p(s)$ for small s, the final estimate in (A1.14) immediately gives

$$A_k(\lambda)\approx 2\sqrt{\pi}(\sinh 2w_c)^{1/2}/(2k)^{3/2}. \tag{A1.15}$$

Thus

$$\tilde{T}_M(x)\approx c_0+2(2\pi/x)(1-x^2)^{1/2}\,\mathrm{e}^{-2Mw_c}/(2M)^{3/2}, \tag{A1.16}$$

which on substitution in (A1.1) immediately yields the results cited in the text. We also note that (A1.16) establishes that the ground state energy per spin (and its relevant derivatives) also converge exponentially.

Appendix A2. Analysis of $S_N(\mu)$

In this appendix we analyse the sum

$$S_N(\mu)=\sum_{k=0}^{N-1}\left[\frac{\mu^2}{N^2}+4\sin^2\left(\frac{\pi k}{N}\right)\right]^{1/2} \tag{A2.1}$$

in the limit $N\to\infty$ with $\mu=0(1)$ using the techniques of Barber and Fisher (1973a) (hereafter denoted BF). Indeed this sum is very similar to one analysed by these authors and thus we only outline the analysis.

Separate off the term $k=0$ and decompose the root as

$$(u^2+v^2)^{1/2}=v[(1+u^2/v^2)^{1/2}-1-u^2/2v^2]+v+u^2/2v, \tag{A2.2}$$

where

$$v=2\sin(\pi k/N), \qquad u=\mu/N. \tag{A2.3}$$

Thus we can write

$$S_N(\mu)=\mu/N+g_1+g_2+g_3, \tag{A2.4}$$

where

$$g_1=4\sum_{k=1}^{[\frac{1}{2}N]}\sin\left(\frac{\pi k}{N}\right)\times\{[1+\mu^2/4N^2\sin^2(\pi k/N)]^{1/2}-1-\mu^2/8N^2\sin^2(\pi k/N)\} \tag{A2.5}$$

$$g_2=2\sum_{k=1}^{N-1}\sin\left(\frac{\pi k}{N}\right) \tag{A2.6}$$

and

$$g_3=\frac{\mu^2}{4N^2}\sum_{k=1}^{N-1}\operatorname{cosec}\left(\frac{\pi k}{N}\right) \tag{A2.7}$$

Note that in g_1 we have reduced the range of the sum to $k\leqslant[\frac{1}{2}N]$, where $[x]$ denotes the largest integer less than or equal to x. This sum can now be analysed for large N as in BF (p24) by (i) replacing sines by their arguments and (ii) extending sums to infinity with the error estimated as in BF. This gives

$$g_1=-\frac{\pi}{N}R_{1\frac{1}{2},0}\left(\frac{\mu^2}{4\pi^2}\right)+O\left(\frac{\mu^2}{N^2}\right), \tag{A2.8}$$

where $R_{1\frac{1}{2},0}(z)$ is the remnant function defined in (4.6).

The sum g_2 can be evaluated exactly:

$$g_2=2\,\mathrm{Im}\sum_{k=1}^{N-1}e^{i\pi kN}=\frac{2\sin(\pi/N)}{1-\cos(\pi/N)}=\frac{4N}{\pi}-\frac{\pi}{3N}+O(N^{-3}). \tag{A2.9}$$

The final sum g_3 is contained in BF (analysed originally by Ferdinand and Fisher (1969)). The essential sum is

$$\sum_{k=1}^{N-1}\operatorname{cosec}\left(\frac{\pi k}{N}\right)=\frac{2N}{\pi}\left[\ln\left(\frac{2N}{\pi}\right)+C_E\right]+O(1), \tag{A2.10}$$

where C_E is Euler's constant. Collecting these results together gives

$$S_N(\mu)=\frac{4N}{\pi}+\frac{2\mu^2}{\pi N}\left[\ln\left(\frac{2N}{\pi}\right)+C_E\right]-\frac{\pi}{2N}R_{1\frac{1}{2},0}\left(\frac{\mu^2}{4\pi^2}\right)+\frac{\mu}{N}-\frac{\pi}{3N}+O(N^{-2}), \tag{A2.11}$$

which is the result quoted in the text.

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