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Finite-size scaling and universality in the (2+1)D Ising model

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Abstract. The energy and magnetisation density of the (2+1)D Ising model are investigated. For the thermal exponent, we find $x_\epsilon = 1.42 \pm 0.02$, in agreement with hyperscaling.

The Privman-Fisher universality hypothesis is confirmed by two methods. First, we present, at the critical point, numerical data for the finite-size scaling amplitudes of the (singular) free energy, magnetisation, susceptibility and surface tension and check them for universality. Second, using the explicitly computed eigenvectors of the Hamiltonian, it is shown that the ratios of matrix elements of the energy and magnetisation density are universal.

1. Introduction

Universality provides the framework for a detailed description of the singular behaviour of statistical systems. This can be expressed most conveniently by the Privman-Fisher (1984) hypothesis which states that the singular part of the free energy density of a system of finite size L should be

$$F^{(s)} = L^{-d} Y(C_1 t L^{1/\nu}, C_2 b L^{\Delta/\nu}) \tag{1.1}$$

where $t = T - T_c$ is the reduced temperature, b is a magnetic field, ν and $\Delta = \beta + \gamma$ are critical exponents and Y is a universal function. All non-universal behaviour can be absorbed into the constants C_1 and C_2. For two-dimensional systems, (1.1) can be obtained as a consequence of conformal invariance (see Reinicke (1987) for a discussion).

In this work we investigate the universality in a three-dimensional Ising model. We shall work with the Hamiltonian (Henkel 1984):

$$H = -h \sum_n \sigma^z(n) - \sum_{(n,n')} \left(\frac{1+\eta}{2} \sigma^x(n)\sigma^x(n') + \frac{1-\eta}{2} \sigma^y(n)\sigma^y(n') \right) \tag{1.2}$$

defined on a square $N \times N$ lattice with periodic boundary conditions. Nearest-neighbour interactions are understood and the σ^x, σ^y, σ^z are the Pauli matrices.

We briefly recall some properties of H (Henkel 1984). At $\eta = 1$, H is the Hamiltonian limit of the 3D Ising model. For each $\eta \neq 0$, there is a critical point falling into the 3D Ising universality class. Some values of the critical field $h_c(\eta)$ are given in

Table 1. Critical point $h_c(\eta)$ and normalisation factor $f(\eta)$. The figures in brackets give the expected uncertainty in the last digit.

η	1.0	0.9	0.7	0.5	0.3
$h_c(\eta)$	3.047 (1)	2.938 (1)	2.720 (1)	2.500 (2)	2.30 (1)
$f(\eta)$	1.0	0.919 (5)	0.752 (5)	0.577 (5)	0.437 (5)

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table 1. H commutes with the operator

$$Q=\frac{1}{2}\left(1-\prod_n \sigma^z(n)\right) \tag{1.3}$$

and the corresponding eigenspaces are called sector 0 and sector 1 according to the eigenvalues of Q. The transverse field h plays the role of the temperature.

Applying finite-size scaling (Fisher 1971, Barber 1983) to H, the critical exponents were obtained for both the triangular (Hamer and Johnson 1986) and the square lattice (Henkel 1984). The results are in excellent agreement with those obtained from the 3D (classical) Ising model (Pawley *et al* 1984, Barber *et al* 1985, Adler 1983, Marland 1981, Le Guillou and Zinn-Justin 1980).

We shall be interested in the universality of the finite-size scaling amplitudes. By universality we mean that the finite-size amplitudes, if H is normalised correctly (see below), are independent of η.

In a recent letter (Henkel 1986), the amplitudes of the energy gaps (or inverse correlation lengths) were studied. It was found that the amplitudes are indeed universal, provided H is renormalised by a factor $1/f(\eta)$ (see table 1). This renormalisation comes from an anisotropic η-dependent rescaling of the 'time' and 'space' directions when performing the τ continuum limit (see, e.g., Kogut 1979) which leads to the quantum Hamiltonian (1.2). The normalisation $f(1)=1$ is chosen for convenience.

We shall extend the above-mentioned study (Henkel 1986) to the energy density operator ε

$$\varepsilon=\frac{1}{\mathcal{N}}\sum_n \sigma^z(n) \tag{1.4}$$

and the magnetisation density operator σ:

$$\sigma=\frac{1}{\mathcal{N}}\sum_n \sigma^x(n) \tag{1.5}$$

($\mathcal{N}=N^2$ is the number of sites) with the scaling dimensions (e.g. Kadanoff 1976)

$$x_\varepsilon=(1-\alpha)/\nu \tag{1.6}$$

$$x_\sigma=\beta/\nu. \tag{1.7}$$

While x_σ was determined earlier to have the value $x_\sigma=0.515\pm0.009$ (Henkel 1984), there exists no finite-size estimate for x_ε in the literature. Conventional finite-size approaches have failed to produce a reliable estimate. We shall show how to overcome this problem and arrive at $x_\varepsilon=1.42\pm0.02$ (see § 2), in agreement with hyperscaling.

We now turn to the universality question. Let $|0\rangle$ be the ground state, $|\varepsilon\rangle$ the first excited state in the sector 0 (whose mass gap is the inverse energy correlation length) and $|\sigma\rangle$ the lowest state in the $Q=1$ sector. Then consider

$$C_{\varepsilon\sigma\sigma}=\frac{\langle\varepsilon|\sigma|\sigma\rangle}{\langle 0|\sigma|\sigma\rangle} \tag{1.8}$$

$$C_{\sigma\varepsilon\sigma}=\frac{\langle\sigma|\varepsilon|\sigma\rangle_{\mathrm{r}}}{\langle 0|\varepsilon|\varepsilon\rangle}. \tag{1.9}$$

(The meaning of the index r will be explained in § 3.)

Both $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$ are found to be independent of η. In contrast to the two-dimensional situation, they are not equal. We shall show, using formal perturbation theory around the critical point Hamiltonian, that this observation of universality

supports the Privman-Fisher hypothesis, not only at the critical point, but for a domain of values of the scaling variables. As a further confirmation of this argument, the Privman-Fisher hypothesis will also be checked directly by comparing the magnetisation and susceptibility amplitudes at the critical point. In addition, we shall also confirm the universality of the singular part of the free energy and also for the surface tension. Similar investigations were done for the (classical) 3D Ising model by Mon (1985) and Mon and Jasnow (1985).

The paper is organised in three large parts. The first part is § 2. We determine x_ε and discuss hyperscaling violations, which have been discussed controversially during recent years. Section 3 is the second part; it contains the investigation of the universality of $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$. We discuss the implications of this result to the Privman-Fisher hypothesis. The last part is made from §§ 4-6. Here we present the numerical evidence which directly supports (1.1). In § 4, we do so by comparing magnetisation and susceptibility amplitudes. In § 5, we study the amplitude of the singular part of the free energy itself and in § 6 we examine the surface tension. In § 7, we present our conclusions. In the appendix, we descibe the numerical methods used for the diagonalisation of H.

2. Determination of the thermal exponent

Before we study the universality of the finite-size scaling amplitudes, we have to determine the exponent x_ε, which is equivalent to a determination (by (1.6)) of α/ν. The conventional approach (Hamer 1983a, Hamer and Johnson 1986) defines the 'specific heat' as

$$c(h) = -\frac{1}{\mathcal{N}} h \frac{\partial^2 E_0(h)}{\partial h^2} \tag{2.1}$$

where E_0 is the ground-state energy of H and $\mathcal{N}$ the number of sites. The application of finite-size scaling to $c(h)$ yields poor results for α/ν (Hamer 1983a, Hamer and Johnson 1986) which deviate by about a factor of two from the results of other methods (see below).

In figure 1, we show $c(h)$ for $\eta = 0.7$ for $N = 2, 3, 4$. It is clearly seen that the maxima of the finite-size specific heat fall quite far from the critical point h_c. This means that the lattices considered are far too small to allow a reliable determination of α/ν from $c(h)$ as defined in (2.1).

We now propose two methods to overcome this problem. They both have in common that one has to compute some *eigenvectors* of the finite-size Hamiltonian. Let $|0\rangle$ denote the ground-state eigenvector and $|\varepsilon\rangle$ the eigenvector of the finite excited state in sector 0. We adopt the following methods.

(i) We compute the matrix element $\langle 0|\varepsilon|\varepsilon\rangle$ of the energy density operator which should scale as (see (1.6))

$$\langle 0|\varepsilon|\varepsilon\rangle \sim N^{-x_\varepsilon}. \tag{2.2}$$

This gives a first recipe to obtain finite-size estimates of x_ε.

(ii) Following the technique of Hamer (1983b), we consider the matrix

$$E = \begin{pmatrix} \langle 0|\varepsilon|0\rangle & \langle 0|\varepsilon|\varepsilon\rangle \\ \langle \varepsilon|\varepsilon|0\rangle & \langle \varepsilon|\varepsilon|\varepsilon\rangle \end{pmatrix}. \tag{2.3}$$

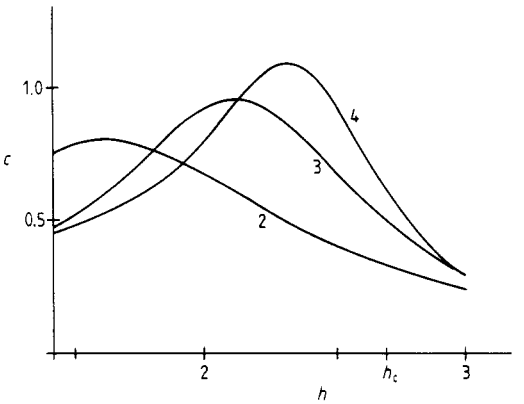

Figure 1. Specific heat for $\eta = 0.7$ as computed from (2.1) for $N = 2, 3, 4$.

Let e_+ be the higher and e_- the lower eigenvalue of E and define the latent heat L per site as

$$L = (e_+ - e_-) \sim N^{-x_\varepsilon} \tag{2.4}$$

and we obtain a second set of estimates for x_ε.

For some values of η, we give $\langle 0|\varepsilon|\varepsilon\rangle$ and L for lattices up to $N = 5$ in table 2. The estimates for x_ε derived from these data and (2.2) and (2.4) are given in table 3. By x_{ε_1}, we denote the estimates obtained from $\langle 0|\varepsilon|\varepsilon\rangle$ and by x_{ε_2} those obtained† from L.

Table 2. Finite-size data for $\langle 0|\varepsilon|\varepsilon\rangle$ and the latent heat L.

	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
N	$\langle 0\|\varepsilon\|\varepsilon\rangle$	L	$\langle 0\|\varepsilon\|\varepsilon\rangle$	L	$\langle 0\|\varepsilon\|\varepsilon\rangle$	L
2	−0.327 35	1.0	−0.302 07	1.0	−0.272 86	1.0
3	−0.211 04	0.524 52	−0.196 29	0.506 06	−0.181 04	0.489 30
4	−0.145 48	0.340 54	−0.136 37	0.325 71	−0.126 91	0.310 72
5	−0.107 35	0.245 06	−0.101 16	0.233 92	−0.094 81	0.222 32

Table 3. Finite-size estimates for the exponent x_ε. In the row labelled $N \to \infty$ we give the van den Broeck-Schwartz approximants for the sequence x_ε defined in the text.

	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
N	x_{ε_1}	x_{ε_2}	x_{ε_1}	x_{ε_2}	x_{ε_1}	x_{ε_2}
3	1.0826	1.5914	1.0631	1.6798	1.0118	1.7629
4	1.2933	1.5015	1.2661	1.5317	1.2349	1.5785
5	1.3621	1.4746	1.3383	1.4836	1.3065	1.5002
$N \to \infty$		1.430		1.421		1.404

† Finite-size estimates $x_\varepsilon(N)$ are obtained from $x_\varepsilon(N) = -\ln(L_N/L_{N-1})/\ln(N/N-1)$ and analogously from $\langle 0|\varepsilon|\varepsilon\rangle$.

We observe that the x_{ϵ_1} form sequences rising with N, while the x_{ϵ_2} sequences are falling with N. We thus expect that the mean $x_\epsilon = \frac{1}{2}(x_{\epsilon_1} + x_{\epsilon_2})$ shows a minimal dependence on N and consequently converges faster than the sequences x_{ϵ_1} and x_{ϵ_2}.

We now want to estimate the limit $N \to \infty$ which is a rather difficult problem with sequences as short as ours. Recall that the critical exponents, which are universal (e.g. Kadanoff 1976), should be independent of η. Looking at the apparent η dependence of the estimated limits gives some idea on the errors involved. Let f_n be a sequence with limit f and define the van den Broeck and Schwartz (1979) approximants $[n, L]$ as follows:

$$[n, -1] = \infty \qquad [n, 0] = f_n \tag{2.5}$$

$$([n, L+1] - [n, L])^{-1} = -a([n, L-1] - [n, L])^{-1} + ([n+1, L] - [n, L])^{-1} + ([n-1, L] - [n, L])^{-1} \tag{2.6}$$

where a is a parameter (for our short sequences and because of (2.5), we can take $a = 0$). The approximants $[n, L]$ are expected to converge faster towards f than the original sequence f_n. For each η, the sequences x_ϵ were extrapolated by the van den Broeck and Schwartz (1979) algorithm and these estimated limits are also given in table 3. Our final estimate for x_ϵ is the mean of these three independent values:

$$x_\epsilon = 1.42 \pm 0.02. \tag{2.7}$$

Using (1.6) and $\nu = 0.629 \pm 0.002$ (Henkel 1984)† we obtain

$$\alpha = 0.11 \pm 0.01. \tag{2.8}$$

This result compares well with those obtained by other methods. Marland (1981) obtained $\alpha = 0.098 \pm 0.003$ from a low-temperature series in the (2+1)D Ising model. In the 3D Ising model, one has $\alpha = 0.12 \pm 0.02$ from high-temperature series (Adler 1983) and $\alpha = 0.110 \pm 0.005$ from the ϕ^4 field theory renormalisation group equation (Le Guillou and Zinn-Justin 1980). This again establishes the universality between the 3D Ising model and its (2+1)D quantum analogue. Thus, comparing with the results from the literature, we can conclude that our approach (2.2) and (2.4) solves the problem of obtaining sensible finite-size estimates for α.

Finally, we briefly discuss hyperscaling. It was suggested by Freedman and Baker (1982) that hyperscaling should be violated in the 3D Ising model. Barber *et al* (1985) have found no sign of hyperscaling violation. For a discussion of possible forms of hyperscaling violation, see Binder *et al* (1985). Using the value $\nu = 0.629 \pm 0.002$ (Henkel 1984), we have the hyperscaling prediction $x_\epsilon = 3 - 1/\nu = 1.410 \pm 0.005$, in excellent agreement with (2.7). We conclude that hyperscaling is satisfied for our model.

3. The amplitudes of the scaling fields

In this section, we first present the numerical evidence for the universality of $C_{\epsilon\sigma\sigma}$ and $C_{\sigma\epsilon\sigma}$ (see (1.8) and (1.9)). Having done this, we discuss the consequences for the Privman-Fisher hypothesis.

† Finite-size estimates for ν can be derived from the beta function and no precise knowledge of the critical point is needed (Hamer 1983a).

3.1. Magnetisation density

Consider the matrix elements of the magnetisation density with the expected scaling behaviour:

$$\langle 0|\sigma|\sigma\rangle = N^{-x_\sigma} a_{0\sigma\sigma}(\eta) \tag{3.1}$$

$$\langle \varepsilon|\sigma|\sigma\rangle = N^{-x_\sigma} a_{\varepsilon\sigma\sigma}(\eta) \tag{3.2}$$

with $x_\sigma = 0.515 \pm 0.009$ (Henkel 1984).

In table 4, we give the amplitudes† $a_{0\sigma\sigma}(\eta)$ and $a_{\varepsilon\sigma\sigma}(\eta)$ for some values of η. The limit $N \to \infty$ is obtained from the van den Broeck and Schwartz (1979) algorithm. Then, we compute $C_{\varepsilon\sigma\sigma}$ from

$$C_{\varepsilon\sigma\sigma} = \lim_{N\to\infty} a_{\varepsilon\sigma\sigma}(\eta)\left(\lim_{N\to\infty} a_{0\sigma\sigma}(\eta)\right)^{-1}. \tag{3.3}$$

From table 4 we see that $C_{\varepsilon\sigma\sigma}$ is independent of η and therefore universal.

3.2. Energy density

For the matrix elements of ε, which are non-diagonal, we expect

$$\langle 0|\varepsilon|\varepsilon\rangle = N^{-x_\varepsilon} a_{0\varepsilon\varepsilon}(\eta) \tag{3.4}$$

with $x_\varepsilon = 1.42(2)$ (see § 2). For the diagonal matrix elements, however, we have

$$\langle \sigma|\varepsilon|\sigma\rangle = a_\varepsilon(\eta) + N^{-x_\varepsilon} a_{\sigma\varepsilon\sigma}(\eta). \tag{3.5}$$

This different scaling behaviour comes from the fact that the operator ε as we wrote it in (1.4) also contains a contribution from the identity operator, which gives rise to the $a_\varepsilon(\eta)$. In order to check that $a_\varepsilon(\eta)$ is really independent of the particular state, we show in figure 2 the three elements $\langle 0|\varepsilon|0\rangle$, $\langle \varepsilon|\varepsilon|\varepsilon\rangle$ and $\langle \sigma|\varepsilon|\sigma\rangle$. We observe that for $N \to \infty$ all three sequences converge towards the same limit.

In order to obtain $a_{\sigma\varepsilon\sigma}(\eta)$ we have to subtract $a_\varepsilon(\eta)$ in (3.5). This leads to the reduced matrix element $\langle \sigma|\varepsilon|\sigma\rangle_r$ mentioned in the introduction. From a computational point of view, the direct subtraction of $a_\varepsilon(\eta)$ is not favourable. Rather, we consider a sequence f_N of the form $f_N = a + bN^{-\omega}$. If ω is known, estimates of b are obtained

Table 4. Finite-size scaling amplitudes $a_{0\sigma\sigma}$ and $a_{\varepsilon\sigma\sigma}$.

	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
N	$a_{0\sigma\sigma}$	$a_{\varepsilon\sigma\sigma}$	$a_{0\sigma\sigma}$	$a_{\varepsilon\sigma\sigma}$	$a_{0\sigma\sigma}$	$a_{\varepsilon\sigma\sigma}$
2	+1.041 78	0.776 99	+1.009 36	0.772 44	+0.974 49	0.772 63
3	+1.062 84	0.853 34	+1.021 07	0.833 19	+0.978 81	0.811 87
4	+1.072 20	0.882 80	+1.027 14	0.855 43	+0.982 19	0.825 67
5	+1.076 49	0.898 75	+1.030 03	0.867 75	+0.984 41	0.832 44
$N \to \infty$	+1.080	0.918	+1.033	0.883	+0.989	0.839
$C_{\varepsilon\sigma\sigma}$		+0.850		+0.855		+0.848

† Since the critical point h_c is not known exactly, this introduces an error $\delta a/a \simeq \delta h_c/h_c \simeq 3 \times 10^{-4}$ which is small compared to the error coming from the extrapolation using (2.5) and (2.6).

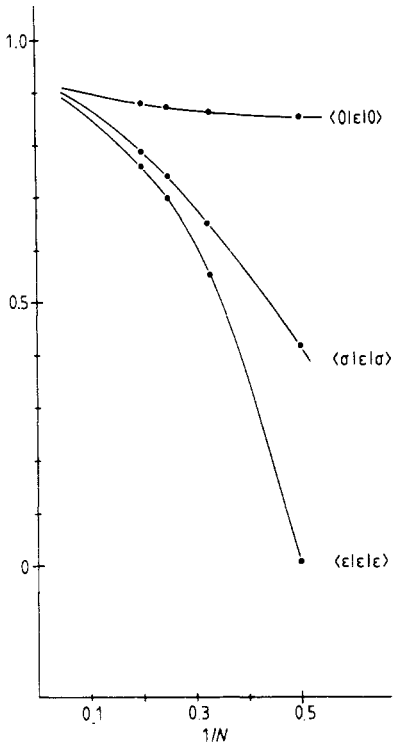

Figure 2. Finite-size estimates for the matrix elements $\langle 0|\varepsilon|0\rangle$, $\langle\sigma|\varepsilon|\sigma\rangle$ and $\langle\varepsilon|\varepsilon|\varepsilon\rangle$. The full curves illustrate the convergence towards a unique limit ($\eta = 1.0$).

from

$$b = \frac{f_{N+1} - f_N}{(N+1)^{-\omega} - N^{-\omega}} \tag{3.6}$$

and no knowledge of a is needed.

In table 5, we give $a_{0\varepsilon\varepsilon}(\eta)$ and $a_{\sigma\varepsilon\sigma}(\eta)$ for some values of η. The limit $N \to \infty$ is obtained with the van den Broeck and Schwartz (1979) algorithm. We then compute

$$C_{\sigma\varepsilon\sigma} = \lim_{N\to\infty} a_{\sigma\varepsilon\sigma}(\eta)\left(\lim_{N\to\infty} a_{0\varepsilon\varepsilon}(\eta)\right)^{-1}. \tag{3.7}$$

Table 5. Finite-size scaling amplitudes $a_{0\varepsilon\varepsilon}$ and $a_{\sigma\varepsilon\sigma}$.

	$\eta = 1.0$		$\eta = 0.7$		$\eta = 0.5$	
N	$a_{0\varepsilon\varepsilon}$	$a_{\sigma\varepsilon\sigma}$	$a_{0\varepsilon\varepsilon}$	$a_{\sigma\varepsilon\sigma}$	$a_{0\varepsilon\varepsilon}$	$a_{\sigma\varepsilon\sigma}$
2	−0.875 94	—	−0.808 29	—	−0.730 13	—
3	−1.004 35	−1.4407	−0.934 15	−1.4505	−0.861 55	−1.4781
4	−1.041 63	−1.2693	−0.976 44	−1.2441	−0.908 67	−1.2224
5	−1.055 18	−1.1992	−0.994 40	−1.1644	−0.931 99	−1.1308
$N \to \infty$	−1.063	−1.15	−1.008	−1.11	−0.955	−1.08
$C_{\sigma\varepsilon\sigma}$		1.08		1.10		1.13

From table 5, we conclude that $C_{\sigma\varepsilon\sigma}$ is universal. Because of the reduction carried out (equation (3.6)), the accuracy of $a_{\sigma\varepsilon\sigma}(\eta)$ is somewhat lower than for the other amplitudes.

Comparing with table 4, we find that $C_{\sigma\varepsilon\sigma}$ and $C_{\varepsilon\sigma\sigma}$ are different. We have considered the possibility of an extremely slow convergence of the estimates of $a_{\sigma\varepsilon\sigma}(\eta)$. Our conclusion is that, although our estimates of $C_{\sigma\varepsilon\sigma}$ might be slightly inaccurate, a possible shift due to a better determination of $a_{\sigma\varepsilon\sigma}(\eta)$ is still not large enough to allow for an equality of $C_{\sigma\varepsilon\sigma}$ and $C_{\varepsilon\sigma\sigma}$.

Our finding contrasts the situation in two dimensions (see, e.g., Cardy 1987), where $C_{\sigma\varepsilon\sigma}$ and $C_{\varepsilon\sigma\sigma}$ are operator product expansion coefficients and therefore automatically equal (von Gehlen *et al* 1987).

3.3. Privman-Fisher hypothesis

We now study the relationship of the universality of $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$ with the Privman-Fisher hypothesis. The Hamiltonian is written as

$$H = H_c + t\sum_n \varepsilon(n) \tag{3.8}$$

where H_c is the critical point Hamiltonian, $t = h - h_c$ and $\varepsilon(n)$ is the local energy density. We stress that ε is the *only* scaling field entering.

As for the two-dimensional case (see Reinicke 1987), we use formal perturbation theory around H_c. In carrying out this formal calculation we use the facts that

(i) the energy gaps at $t = 0$, $b = 0$ are universal (Henkel 1986),

(ii) $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$ are universal,

(iii) the hyperscaling relation $d - x_\varepsilon = 1/\nu$ is valid.

It follows that the Privman-Fisher hypothesis (1.1) is supported not only for $t = 0$ but for a domain of values of the scaling variable $z = tN^{1/\nu}$ (in the limit $t \to 0$, $N \to \infty$ such that z is kept fixed).

In exactly the same way one can treat a magnetic field $b\,\Sigma_n \sigma^x(n)$.

For a different approach towards the scaling function using ε-expansion techniques, see Brézin (1982) and Brézin and Zinn-Justin (1985).

4. Magnetisation and susceptibility amplitudes

In this and the following sections, we proceed to test the Privman-Fisher hypothesis directly at the critical point. The eventual verification provides additional evidence independent of the reasoning of § 3.

We begin by comparing the magnetisation and susceptibility amplitudes. At $h = h_c(\eta)$, the free energy density is

$$F^{(s)} = N^{-d} f(\eta)\, Y(0, C_2(\eta) b N^{\Delta/\nu}) \tag{4.1}$$

and we have included explicitly the normalisation constant $f(\eta)$. For the magnetisation and susceptibility densities at the critical point we have

$$M = N^{-\beta/\nu} f(\eta) C_2(\eta)\, Y'(0,0) = N^{-\beta/\nu} a_M(\eta) \tag{4.2}$$

$$\chi = N^{\gamma/\nu} f(\eta) C_2^2(\eta)\, Y''(0,0) = N^{\gamma/\nu} a_\chi(\eta) \tag{4.3}$$

where a prime denotes differentiation with respect to b. Consequently, we expect that the quantity $a_M^2/(a_\chi(\eta) f(\eta))$ is universal.

Table 6. Finite-size scaling susceptibility amplitude a_χ.

N	$a_\chi(1.0)$	$a_\chi(0.7)$	$a_\chi(0.5)$
2	0.4527	0.6117	0.8155
3	0.4983	0.6221	0.7680
4	0.5183	0.6346	0.7660
$N\to\infty$	0.52	0.64	0.76
$a_M^2/(a_\chi f)$	2.24	2.21	2.21

Finite-size magnetisations can be computed, using Yang's (1952) trick, from (Hamer 1982)

$$M = \langle 0|\sigma|\sigma\rangle. \tag{4.4}$$

The amplitude $a_M = a_{0\sigma\sigma}$ can be taken from table 4. In table 6, we show the amplitudes of the finite-size susceptibility (from the scaling relations and x_ε and x_σ, we have $\gamma/\nu = 1.97$). We take the values for $N = 4$ to estimate the limit $N\to\infty$ of a_χ.

We conclude from the data of table 6 that $a_M^2/(a_\chi(\eta)f(\eta))$ is indeed universal, in agreement with the Privman-Fisher (1984) hypothesis.

5. Universality of the free energy

We now consider the free energy density at the critical point. It is well known that the free energy contains a singular term (which gives rise to the singularity of the specific heat) and a regular term (proportional to the volume of the system). For periodic boundary conditions, we expect for the free energy density the scaling behaviour:

$$F = F^{(r)} + N^{-d}a_F \tag{5.1}$$

where $F^{(r)}$ comes from the regular part and is non-universal.

In order to check the universality of a_F, we again use (3.6). In table 7, we give the estimates for a_F. We have to take into account the η-dependent renormalisation of the Hamiltonian, as mentioned in the introduction. We therefore give in the last row of table 7 the renormalised amplitudes $a_F(\eta = 1.0)f(\eta)$ and compare them with the a_F obtained from (5.1). The values for $f(\eta)$ are from table 1.

We conclude that universality holds. Mon (1985) computed, for the 3D (classical) Ising model, the amplitude a_F for the SC and BCC lattice and obtained universality with respect to the lattice type.

Table 7. Finite-size scaling amplitudes a_F of the singular part of the free energy.

N	$\eta = 1.0$	$\eta = 0.9$	$\eta = 0.7$	$\eta = 0.5$	$\eta = 0.3$
3	1.5240	1.3018	0.8829	0.5072	0.1988
4	1.3820	1.2485	0.9653	0.6618	0.3383
5	1.2990	1.1808	0.9536	0.7033	0.4311
$N\to\infty$	1.18	1.0	0.91	0.72	0.54
$a_F(1.0)f(\eta)$	1.18	1.08	0.89	0.68	0.52

6. Surface tension

As a last topic, we study the surface tension at the critical point. Let $E_0^{(a)}$ be the ground-state energy of H (equation (1.2)) with antiperiodic boundary conditions in *both* directions and $E_0^{(p)}$ is the same quantity with periodic boundary conditions. Then the surface tension τ is defined as

$$\tau = E_0^{(a)} - E_0^{(p)}. \tag{6.1}$$

Our definition is different from the usual one (e.g. Widom 1972, Mon and Jasnow 1985) since we have antiperiodic boundary conditions in *two* instead of one dimensions. We expect a finite-size scaling behaviour

$$\tau = \tau_0(\eta) N^{-1}. \tag{6.2}$$

In table 8, we give the finite-size estimates for $\tau_0(\eta)$. Since the sequences are not always monotonic, the van den Broeck-Schwartz (1979) algorithm does not work for $\eta = 0.5$ and $\eta = 0.3$. For $\eta = 0.3$, we used linear extrapolation instead, while for $\eta = 0.5$ the given limit depends on our feeling how far the curve will go down, as determined in the $\eta = 0.7$ case.

Table 8. Finite-size scaling amplitudes τ_0 of the surface tension.

N	$\eta = 1.0$	$\eta = 0.9$	$\eta = 0.7$	$\eta = 0.5$	$\eta = 0.3$
2	2.984 37	2.575 74	1.798 82	1.093 23	0.482 06
3	2.547 46	2.306 84	1.800 95	1.265 87	0.672 53
4	2.340 64	2.140 02	1.726 00	1.292 70	0.754 26
5	2.241 22	2.055 63	1.676 17	1.291 10	0.781 07
$N \to \infty$	2.149	1.969	1.577	1.2	0.9
$\tau_0(1.0) f(\eta)$	2.149	1.975	1.616	1.240	0.939

To check for universality, we note that because of (6.1), $\tau_0(\eta)$ still contains the renormalisation factor $f(\eta)$. In the last row of table 8, we show the renormalised amplitudes $\tau_0(1.0)\, f(\eta)$ and find that they agree with $\tau_0(\eta)$. So we can conclude that the finite-size scaling amplitude of the surface tension is universal.

Our result is a counterpart to the work of Mon and Jasnow (1985) who studied, for the 3D Ising model, the surface tension on lattices with antiperiodic boundary conditions in only one direction.

The universality of the amplitude of the surface tension can also be looked at in a different way. From (6.1), τ is the difference of the free energies computed with antiperiodic and periodic boundary conditions. The leading non-universal terms in N of $E_0^{(a)}$ and $E_0^{(p)}$ cancel since they must not depend on the boundary conditions. Consequently, τ_0 measures the difference of the amplitudes a_F of the singular part of the two free energies. From § 5 we know that the amplitudes a_F of the singular part are universal for periodic boundary conditions. It follows that the amplitude with antiperiodic boundary conditions is also universal.

Together with the verification for the correlation lengths (Henkel 1986), this is the first verification of the Privman-Fisher hypothesis for non-periodic boundary conditions in the three-dimensional Ising model.

7. Discussion

We have studied, as a prototype of three-dimensional critical behaviour, a set of models lying in the 3D Ising universality class. We expect that the general universality features found will also be valid for other models.

We have concentrated our attention on the verification of the Privman-Fisher (1984) hypothesis, which dictates how non-universal behaviour can enter into the finite-size scaling function at all.

By direct computation at the critical point, we have verified the Privman-Fisher hypothesis for the following physical quantities:

(1) the correlation length (Henkel 1986),
(2) the magnetisation,
(3) the susceptibility,
(4) the (singular) free energy,
(5) the surface tension.

The confirmation of (4) and (5) is further supported from the independent work of Mon (1985) and Mon and Jasnow (1985). The agreement of their results and ours supports the universality between the 3D and the (2+1)D Ising model. We also confirmed (1) and (4) for antiperiodic boundary conditions.

Specific to the Hamiltonian approach used is the possibility to compute the eigenvectors (and not only eigenvalues, which correspond to ensemble averages) of the Hamiltonian. This offers new ways of investigation.

(*a*) We have been able, for the first time, to obtain reliable finite-size estimates for the exponent x_ε (1.6):

$$x_\varepsilon = 1.42 \pm 0.02 \tag{7.1}$$

which is in agreement with hyperscaling. This result does not agree with the observation of a hyperscaling violation in the 3D Ising model by Freedman and Baker (1982).

(*b*) The quantities $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$ (equations (1.8) and (1.9)) were shown to be universal. This result can be used to support the Privman-Fisher (1984) hypothesis not only at the critical point itself but for a domain of values of the scaling variables.

Although this general feature looks similar to the situation in two dimensions, an important difference is that the numbers $C_{\varepsilon\sigma\sigma}$ and $C_{\sigma\varepsilon\sigma}$ appear not to be equal. It would be desirable to be able to use larger lattices than 5×5 (which already involves $86\,056\times86\,056$ matrices) in order to clarify this point further.

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Appendix. Numerical methods

We describe the numerical techniques for the calculation of eigenvalues and eigenvectors of the 5×5 lattice. We consider both periodic and antiperiodic boundary conditions.

We utilise the invariance of H under rotations, reflections and translations. Rotations and reflections can be treated exactly the same way for both types of boundary conditions. For antiperiodic boundary conditions, however, the translation operators T_x and T_y generating translations parallel to the x axis and y axis, repectively, do not commute with H. Instead, we take in this case

$$\tilde{T}_x = \left(\prod_{r=0}^{N-1} \sigma^z(1, Nr+1) \right) T_x \tag{A1}$$

$$\tilde{T}_y = \left(\prod_{r=0}^{N-1} \sigma^z(Nr+1, 1) \right) T_y. \tag{A2}$$

It is a straightforward exercise to show that $\tilde{T}_x$ and $\tilde{T}_y$ commute with H for antiperiodic boundary conditions. The states $|\psi\rangle$ are now cast into invariance classes $|\psi)$ labelled by some representative ψ. The computation of the elements of H on the classes $|\psi)$ is done in three steps.

(i) Determination of the representatives and the number of elements of the invariance classes as follows: each configuration of the lattice is given by an integer between 0 and $2^{25}-1$ from its binary representation. The smallest configuration of an invariance class is chosen as its representative. Starting with the configuration 0, each configuration will be transformed by all symmetry transformations of the lattice. If one obtains a configuration in this way which is smaller than the one started from, the starting configuration must be a member of a class already considered. After at most 2^{24} configuration the procedure is finished, the only missing configuration being $2^{25}-1$.

(ii) Computation of the diagonal elements.

(iii) The off-diagonal elements are computed from

$$(\varphi|H|\psi) = \left(\frac{n}{m}\right)^{1/2} \sum_r \sum_\tau \langle\varphi|T^r|\tau\rangle\langle\tau|H|\psi\rangle \tag{A3}$$

where the class $|\varphi)$ has m elements and $|\psi)$ has n elements and T stands for any one of the symmetry operators.

This method is convenient since it allows an efficient computation of the elements of both σ^x and σ^y. All that is needed to store is whether H flips a pair of parallel or antiparallel spins.

For the 5×5 lattice, we have 86 056 invariance classes. For each charge sector one needs 27 Mbytes of storage for the matrix elements.

The computations were carried out on a VAX 11/780. Steps 1 and 2 for both sectors together took 3.5 h CPU time (for the sector 0, the results can also be used for antiperiodic boundary conditions), step 3 took 11.5 h for each sector for periodic boundary conditions and 13 h for antiperiodic boundary conditions.

The eigenvalues were computed using the Lanczos (1950) algorithm. For 25 iteration steps, which give the eigenvalues to about ten digits accuracy, we needed about 50 min CPU time.

To obtain the eigenvectors, we first applied about 200 iterations of the BMKD algorithm (Berger *et al* 1977), which produces extremely stable results. The BMKD algorithm only gives the lowest eigenvalue and the corresponding eigenvector. To obtain the eigenvector $|\varepsilon\rangle$ of the second level in the sector 0, we used the resulting vector of the BMKD scheme, which gave the eigenvalue with an accuracy better than 10^{-6}, as a starting vector for an additional run of six Lanczos iterations.

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