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Finite size scaling and crossover phenomena: the *XY* chain in a transverse field at zero temperature

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Abstract. The scaling theory of finite size effects in the limiting bulk behaviour is extended to treat crossover phenomena. The method is used to study quantum critical phenomena in the *XY* chain in a transverse field at zero temperature, through the scaling of the longitudinal susceptibilities and of the energy gaps between the ground and two first excited states. As expected, no abrupt change in critical exponents is observed for small anisotropy, because of the finiteness of the system, but the limiting isotropic and anisotropic regions display quite distinct critical behaviour, in good agreement with known results. Another interesting result obtained is that the two energy gaps examined vanish at the critical line with the same critical exponent.

1. Introduction

The understanding of critical phenomena has developed a great deal during the last two decades, in particular with the ideas of universality (Kadanoff 1975) and the renormalisation group (Wilson and Kogut 1974, Wallace and Zia 1978).

The universality hypothesis states that systems exhibiting critical behaviour can be cast into universality classes, determined by the lattice and order parameter dimensionalities only, provided the interactions are short ranged (Kadanoff 1975). In this way, if the dimensionality of the order parameter changes due to, say, exchange anisotropy, the critical behaviour crosses over to a different one. Crossover phenomena have been investigated with the aid of scaling functions (Riedel and Wegner 1969, Pfeuty *et al* 1974) as well as with the renormalisation group (RG) (see Aharony 1976).

On the other hand, the ideas of scaling have been used to investigate the asymptotic behaviour of systems of large but finite sizes and thin films, with the finite size scaling (FSS) hypothesis (Fisher 1971, Suzuki 1977), which can be though of as a theory of crossover between finite and infinite size behaviours. The central assumption behind this hypothesis is the existence of a single diverging correlation length when the system becomes infinitely large (Fisher 1971). As a consequence, the class of systems described by the FSS hypothesis as it stands (Fisher 1971) is restricted to those with a single diverging correlation length, although there may be more than one relevant variable (in the RG sense), such as in an Ising magnet with a longitudinal field. The FSS treatment of crossover phenomena with more than one diverging correlation length is therefore ruled out.

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The purpose of this work is to extend the original FSS theory (Fisher 1971) to treat crossover phenomena and to illustrate its use by treating a problem in quantum critical phenomena.

To this end §§ 2 and 3 briefly review finite size (Fisher 1971) and crossover (Pfeuty *et al* 1974) scaling theories, respectively. In § 4 we introduce the extended finite size scaling (EFSS) ansatz, and analyse its properties. In § 5 we apply these ideas to the anisotropy exchange in the one-dimensional XY model with a transverse field at zero temperature. Section 6 closes this paper with discussions of the scope and limitations of the EFSS hypothesis.

2. Finite size scaling

FSS theory was developed by Fisher and co-workers (see Fisher 1971) in order to study the approach to criticality for systems of large but finite extension in one or more spatial dimension.

Consider for simplicity a d-dimensional hypercubic lattice with n spins along each one of its directions, with nearest-neighbour coupling g. When n is kept finite there are two competing characteristic lengths for this system, namely the size n and the limiting (i.e. $n \to \infty$) correlation length ξ supposed to behave as

$$\xi \sim |g - g_c|^{-\nu} \tag{2.1}$$

for g near the critical value g_c. In this way, if n is finite and $g \simeq g_c$, order cannot build up beyond distances of the order n: the limiting critical behaviour is inhibited. When $n \to \infty$, on the other hand, order can have infinite range.

Based on these observations, the asymptotic behaviour of a quantity X_n (such as susceptibility, specific heat or the correlation length), calculated for a system of (large) size n and for g near g_c, is given by the FSS hypothesis (Fisher 1971)

$$X_n(g) \simeq n^{x/\nu} Q(y) \tag{2.2}$$

where

$$y \equiv n/\xi. \tag{2.3}$$

x is the exponent characterising the limiting behaviour of X_n, i.e.

$$\lim_{n \to \infty} X_n(g) \sim |g - g_c|^{-x} \tag{2.4}$$

for g near g_c, and $Q(y)$ is the finite size scaling function with the properties (Fisher 1971)

$$Q(y) \sim \begin{cases} \text{constant} & \text{for } y \to 0, \\ y^{-x/\nu} & \text{for } y \to \infty. \end{cases} \tag{2.5}$$

As discussed by Fisher (1971), one might prefer to scale with the variable

$$\dot{y} \equiv n^{1/\nu}[(g - g_c(n))/g_c(\infty)] \tag{2.6}$$

which introduces the pseudo-critical coupling $g_c(n)$ as the point at which $X_n(g)$ has a maximum (rounded-off singularity). Also, if we allow the system to be actually infinite in $d' < d$ dimensions but of finite size n in the remaining ones, then $g_c(n)$ is an actual critical point, characterising d'-dimensional critical behaviour. The use of $\dot{y}$ allows the asymptotic behaviour of $g_c(n)$ to be determined, unlike y which predicts a special dependence on n for $g_c(n)$ (Fisher 1971). Provided we are not interested in the actual n-dependence of the pseudo-critical coupling, we can use the unshifted reduced variable y.

The FSS hypothesis, as given by (2.2) with (2.3) or (2.6), has been confirmed by several calculations on Ising and spherical models (reviewed by Fisher (1971)), on the transverse Ising model at zero temperature (Hamer and Barber 1981, dos Santos 1980) and on the isotropic Heisenberg model (Ritchie and Fisher 1973).

The assumption of a single relevant correlation length rules out any possibility of the hypothesis (2.2) describing crossover phenomena, since these are usually characterised by the existence of more than one diverging correlation length, as discussed in the next section.

3. Crossover phenomena

For the sake of simplicity let us restrict ourselves to spin Hamiltonians of the type

$$H = H_I(g) + \eta H_A(g) \tag{3.1}$$

where the subscripts I and A stand for isotropic and anisotropic respectively, g is a coupling constant and η measures the anisotropy and may be assumed to vary between 0 and 1. Let us further assume that the system described by (3.1) becomes critical as one crosses a critical line $g_c(\eta)$.

In the cases where H_A has a lower symmetry than H_I, it follows from the universality hypothesis that the isotropic critical behaviour crosses over to the anisotropic critical behaviour even for a small degree of anisotropy. This means that for fixed η a thermodynamic quantity $X(g, \eta)$ (e.g. susceptibility, specific heat, magnetisation, correlation length, etc) behaves like

$$X(g, \eta) \sim \begin{cases} |g - g_c(0)|^{-x_0} & \text{for } \eta = 0, \\ |g - g_c(\eta)|^{-x} & \text{for } \eta > 0, \end{cases} \tag{3.2}$$

for $|g - g_c(\eta)|$ small enough, where x and x_0 are in general different.

Riedel and Wegner (1969) introduced a crossover scaling theory in which they assumed that the quantity X above can be given by

$$X(g, \eta) = \dot{t}^{-x_0} F(\eta / \dot{t}^{\phi}) \tag{3.3}$$

where

$$\dot{t} = (g - g_c(\eta)) / g_c(0) \tag{3.4}$$

is the shifted reduced coupling, ϕ is the crossover exponent and the function $F(z)$ has the properties

$$F(z) \sim \begin{cases} \text{constant} & \text{for } z \ll 1, \\ z^{(x - x_0)/\phi} & \text{for } z \gg 1. \end{cases} \tag{3.5}$$

The region $z \sim 1$ is called the crossover region in the sense that for $g \leqslant g^{\times}$, where

$$g^{\times} = g_c(\eta) + A\eta^{1/\phi} \tag{3.6}$$

and A is a constant, the effects of anisotropy begin to dominate the isotropic behaviour.

An extended scaling theory was discussed by Pfeuty *et al* (1974) in which the above mentioned quantity X scales like

$$X(g, \eta) = t^{-x_0} F_0(\eta/t^{\phi}) \tag{3.7}$$

where we note the appearance of the reduced coupling

$$t = (g - g_c(0))/g_c(0) \tag{3.8}$$

instead of the shifted reduced coupling (3.4).

While the form (3.3) leaves open the question about the shift exponent ψ, defined through

$$g_c(\eta) \sim g_c(0)(1 + w\eta^{1/\psi}) \tag{3.9}$$

for small η, the extended scaling form (3.7) necessarily implies $\psi = \phi$ (Pfeuty *et al* 1974). The same point, with η replaced by $1/n$ where n is the size of a finite system, appears in conjunction with the FSS hypothesis (Fisher 1971).

The asymptotic behaviour of $F_0(z)$ is now given by (Pfeuty *et al* 1974)

$$F_0(z) \sim \begin{cases} \text{constant}, & z \ll 1, \\ (z - z_c)^{-x}, & z \to z_c, \end{cases} \tag{3.10}$$

where z_c is related to $g_c(\eta)$.

If one takes the derivative of X as given by (3.7) with respect to η at $\eta = 0$, it is easy to show that it behaves like

$$\partial X/\partial \eta|_{\eta=0} \sim t^{-(x_0+\phi)} \tag{3.11}$$

so that the logarithmic derivative of X behaves like

$$\partial/\partial\eta \ln X|_{\eta=0} \sim t^{-\phi} \tag{3.12}$$

which may be used to calculate the crossover exponent ϕ (Pfeuty *et al* 1974).

The EFFS hypothesis must allow for the possibility of more than one correlation length diverging. In particular, for the anisotropy crossover we can define two correlation lengths ξ_1 and ξ_2 in such a way that for $\eta = 0$ both ξ_1 and ξ_2 diverge at $g_c(0)$, whereas for $\eta > 0$ only one, say ξ_2, diverges at $g_c(\eta)$, the other one remaining finite. We may write, using the extended scaling form,

$$\xi_1 = t^{-\nu_0} F_1(\eta/t^{\phi}) \tag{3.13}$$

and

$$\xi_2 = t^{-\nu_0} F_2(\eta/t^{\phi}) \tag{3.14}$$

where $F_1(z)$ and $F_2(z)$ have the asymptotic forms

$$F_1(z) \sim \begin{cases} A & \text{as } z \to 0, \\ B & \text{as } z \to z_c, \end{cases} \tag{3.15}$$

where A and B are constants and

$$F_2(z) \sim \begin{cases} A & \text{as } z \to 0, \\ (z - z_c)^{-\nu} & \text{as } z \to z_c. \end{cases} \tag{3.16}$$

4. The extended finite size scaling hypothesis

Let us now consider a d-dimensional hypercube of finite extent n in all its dimensions.

If we want to allow for the possibility of crossover phenomena to occur in the thermodynamic limit, we must introduce a second variable into the usual FSS hypothesis. The discussion in the previous section then suggests that for a finite system it is the competition between n/ξ_1 and n/ξ_2 for fixed g and η that will determine which critical behaviour will occur when we take the thermodynamic limit.

Thus, the thermodynamic quantity $X(g, \eta)$, whose critical behaviour in the thermodynamic limit was discussed in § 3, is assumed to behave for a system with finite (but large) size n as

$$X_n(g, \eta) \approx n^{\omega} Q(n/\xi_1, n/\xi_2) \tag{4.1}$$

where ω is a constant to be determined, and $Q(u, v)$ is the extended finite size scaling function.

There are some conditions to be imposed on the asymptotic behaviour of $Q(u, v)$. Firstly, for fixed g and η such that g is near $g_c(\eta)$ we must reproduce the crossover scaling form (3.7) when $n \to \infty$. For this we may assume that

$$Q(u, v) \xrightarrow[u,v\to\infty]{} u^{-\omega} \Phi(u/v) \tag{4.2}$$

in order to cancel any n-dependence, with Φ being some function of $y = u/v = \xi_1/\xi_2$. Further, with equations (3.13) and (3.14) we can write (4.2) as

$$Q(u, v) \xrightarrow[u,v\to\infty]{} n^{-\omega} t^{-\omega\nu_0} F(\eta/t^{\phi}) \tag{4.3}$$

where

$$F(z) = F_1^{\omega}(z) \Phi[F_1(z)/F_2(z)] \tag{4.4}$$

so that

$$X(g, \eta) = \lim_{n\to\infty} X_n(g, \eta) = t^{-\omega\nu_0} F(z). \tag{4.5}$$

Comparing (4.5) with (3.7), we obtain

$$\omega = x_0/\nu_0. \tag{4.6}$$

The second requirement upon Q concerns the recovery of the usual FSS ansatz for *fixed* η. Thus, for finite n and fixed $\eta = 0$, $\xi_1 = \xi_2$, so that

$$X_n(g) = n^{x_0/\nu_0} R(n/\xi_2) \tag{4.7}$$

where $R(n/\xi_2) = Q(n/\xi_2, n/\xi_2)$. On the other hand, for finite n and fixed $\eta > 0$ we must assume that for g sufficiently close to $g_c(\eta)$ the function Q is separable, i.e.

$$Q(u, v) \sim S(u) T(v), \tag{4.8}$$

in order to preserve the n-dependence and recover the usual FSS ansatz, with S and T being scaling functions of their variables. Further, as for $\eta > 0$ ξ_1 is a well behaved function of η (cf equations (3.13) and (3.15)) we may write $u \sim nf(\eta)$ and we may expect

$$S(u) \sim u^{\varepsilon} \sim [nf(\eta)]^{\varepsilon} \tag{4.9}$$

to leading order in n, with ε to be determined.

We can finally write for $\eta > 0$

$$X_n(g, \eta) \approx n^{x/\nu}[f(\eta)]^{\varepsilon} T(n/\xi_2) \tag{4.10}$$

with

$$\varepsilon = x/\nu - x_0/\nu_0 \tag{4.11}$$

to be consistent with the usual FSS hypothesis.

It is worth stressing that equation (4.9) is only valid for $n \gtrsim \xi_1(g, \eta)$, which means that the expected discontinuity at $\eta = 0$ in the n-exponent only takes place as $n \to \infty$. For $n < \xi_1(g, \eta)$ near the unstable critical point $(g_c(0))$ the system behaves only slightly differently.

The simplest test of these ideas is to plot $\ln X_n[g_c(\eta)]$ against $\ln n$ for various η and examine the trend of the slopes of these curves for different values of η. Moreover, we can define successive estimates $\psi_n(\eta)$, for the n-exponent in the EFSS hypothesis as the slope of the straight line joining $\ln X_{n+1}(g_c(\eta), \eta)$ to $\ln X_n(g_c(\eta), \eta)$:

$$\psi_n(\eta) \equiv \frac{\ln X_{n+1}(g_c(\eta), \eta) - \ln X_n(g_c(\eta), \eta)}{\ln (n+1/n)} \tag{4.12}$$

which should yield

$$\psi_n(0) \to x_0/\nu_0 \qquad \text{as } n \to \infty, \tag{4.13}$$

$$\psi_n(\eta) \to x/\nu \qquad \text{as } n \to \infty. \tag{4.14}$$

The ratio ϕ/ν_0 can also be estimated by a similar procedure: taking the derivative of X_n with respect to η at $\eta = 0$ and using (3.11) for $\partial\xi_2/\partial\eta|_{\eta=0}$, we obtain

$$\partial X_n/\partial\eta|_{\eta=0} \approx n^{1+x_0/\nu_0} t^{\nu_0-\phi} Z(n/t^{-\nu_0}) \tag{4.15}$$

where Z is some function of the scaling variable nt^{ν_0}, which implies

$$\partial(\ln X_n)/\partial\eta|_{\eta=0} \sim nt^{\nu_0-\phi} Y(n/t^{-\nu_0}) \tag{4.16}$$

where we use the fact that for $\eta = 0$

$$\xi_1 = \xi_2 \approx t^{-\nu_0}. \tag{4.17}$$

The function $Y(u_0)$, with $u_0 = n/\xi_2$ for $\eta = 0$ (cf equations (3.16) and (4.7)), has the properties

$$\lim_{u_0 \to \infty} Y(u_0) \sim u_0^{-1} \tag{4.18}$$

in order to cancel the residual n-dependence and

$$\lim_{u_0 \to 0} Y(u_0) \sim u_0^{\phi/\nu_0 - 1} \tag{4.19}$$

in order to avoid the possibility of singular behaviour for finite n as $t \to 0$. With (4.19) we have from (4.16)

$$\ln \left(\frac{\partial}{\partial\eta} \ln X_c[g_c(\eta)] \bigg|_{\eta=0} \right) \approx \frac{\phi}{\nu_0} \ln n \tag{4.20}$$

so that the ratio ϕ/ν_0 is given as the slope of a log–log plot of the logarithmic derivative of X with respect to η at $\eta = 0$ against n.

Another test of the scaling hypothesis presented here is to plot $n^{-x/\nu}X_n[g_c(\eta)]$ against η which, according to equation (4.10), should be independent of n away from the crossover region.

In the following section we apply these ideas to anisotropy crossover in the one-dimensional transverse XY model at zero temperature.

5. The anisotropy crossover in the one-dimensional XY model in a transverse field at zero temperature

The simplest system exhibiting crossover that is amenable to test the EFSS hypothesis is the one-dimensional spin-$\frac{1}{2}$ transverse XY model (TXYM [1]) at zero temperature. Its Hamiltonian is

$$H = -\Gamma \sum_i \sigma_i^z - \tfrac{1}{2}J(1+\eta)\sum_i \sigma_i^x\sigma_{i+1}^x - \tfrac{1}{2}J(1-\eta)\sum_i \sigma_i^y\sigma_{i+1}^y \tag{5.1}$$

where Γ is the transverse field, J is the exchange interaction, η measures the anisotropy and σ^α ($\alpha = x, y, z$) are Pauli spin matrices. Note that H is invariant with respect to the interchange $\eta \to -\eta$, $\sigma^x \to \sigma^y$, $\sigma^y \to -\sigma^x$. For any $|\eta| > 0$ the system becomes critical at $g_c \equiv (\Gamma/J)_c = 1$, with the same critical exponents as for the transverse Ising model ($|\eta| = 1$) (Katsura 1962, Barouch and McCoy 1971, Suzuki 1971). For $\eta = 0$, although there is no long-range order (Vaidya and Tracy 1978, Jullien and Pfeuty 1979) the longitudinal susceptibilities χ^{xx} and χ^{yy} as well as the correlation lengths related to the correlation functions $\langle 0|\sigma_0^x\sigma_r^x|0\rangle$ and $\langle 0|\sigma_0^y\sigma_r^y|0\rangle$ are observed to diverge also at $g_c = 1$, but with exponents different from the anisotropic case (Barouch and McCoy 1971, Gerber and Beck 1977, Jullien and Pfeuty 1979). The fact that the critical line is then known in the thermodynamic limit to be $g_c(\eta) = 1$ is helpful in testing the effects of crossover in a TXYM [1] system of finite size.

Before carrying out such a test we must first discuss the general features of the thermodynamic quantities used in our calculations.

5.1. Low-lying energy gaps

The nature of the low-lying excitation spectrum of the Hamiltonian (5.1) can be discussed qualitatively by following the lines of the perturbative approach used by Pfeuty and Elliott (1971) for the transverse Ising model.

Consider first $\eta = 1$ and let us look at two limiting cases: Ising model ($\Gamma = 0$) and independent spins ($J = 0$). When $\Gamma = 0$ the ground state is doubly degenerate due to the discrete symmetry ($\sigma^z \to -\sigma^z$), and the first excited state (corresponding to all spins to one side of the given spin being flipped) is N-fold degenerate, where N is the number of spins. When a small transverse field is switched on, the latter degeneracy is lifted, giving rise to a continuous band of excited states when $N \to \infty$. On the other hand, when $J = 0$ the ground state is a singlet, but the first excited state is also N-fold degenerate. Again, when a small Ising interaction is switched on, the degeneracy is lifted, giving rise for an infinite system, to a continuous band of excited states. At the critical point $(\Gamma/J)_c$ there is then a change in the degeneracy of the ground state. Moreover, according to the results of Pfeuty (1970) and Pfeuty and Elliott (1971), the energy gap between the two lowest states vanishes as the critical point is approached both from above and below. Since the excited states form a continuum we can expect that the energy gap between the ground and second excited states also vanishes at $(\Gamma/J)_c$. If we denote these two energy gaps mentioned above by Δ and $\tilde{\Delta}$ respectively, we may assume that for $g(\equiv\Gamma/J)$ near g_c we have

$$\Delta \sim |g - g_c|^s \tag{5.2}$$

and

$$\tilde{\Delta} \sim |g - g_c|^{\tilde{s}} \tag{5.3}$$

where in principle the gap exponents s and $\tilde{s}$ are different.

The above arguments can be equally applied to the low-lying spectrum for $0 < \eta < 1$, and we expect the same behaviour as (5.2) and (5.3) with g_c being replaced by $g_c(\eta)$. Moreover, for $\eta = 0$ a similar reasoning is also valid, with the proviso that for the low field phase the ground state has a continuous symmetry. We can also expect the gaps to behave as (5.2) and (5.3) but with g_c, s and $\tilde{s}$ being replaced by $g_c(0)$, s_0 and $\tilde{s}_0$, respectively.

Moreover, the dynamical critical exponent (Hohenberg and Halperin 1977) at zero temperature is given by the ratio between the gap exponent s (or s_0) and the correlation length exponent ν (or ν_0), which is exactly the exponent of n in the FSS hypothesis. Within the EFSS approach, we are then able to investigate the crossover in the dynamic critical behaviour at zero temperature, by defining the dynamical exponent as

$$z = s/\nu, \qquad z_0 = s_0/\nu_0, \tag{5.4}$$

and extending this definition to the gap $\tilde{\Delta}$ as

$$\tilde{z} = \tilde{s}/\nu, \qquad \tilde{z}_0 = \tilde{s}_0/\nu_0. \tag{5.5}$$

In figure 1 we show log–log plots of Δ and $\tilde{\Delta}$ at $g = 1$ for various values of η as a function of the size n of a chain with free ends. Note that as η goes from 0 to 1, the

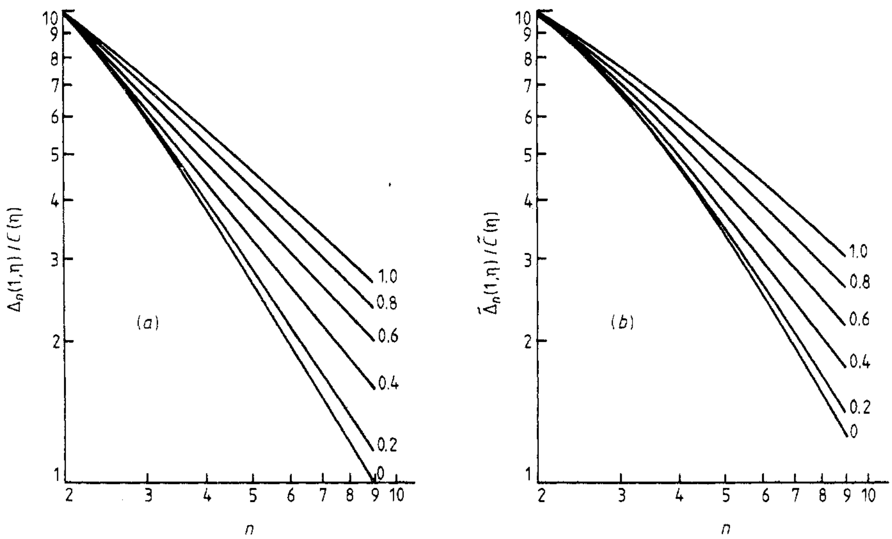

Figure 1. Normalised energy gaps between the ground state and both the first (a) and the second (b) excited states as functions of n at constant anisotropy η, for chains with free ends. The curves are labelled by the values of η.

exponents z and $\tilde{z}$ as given by the slopes of the log–log plots go from ~2 to ~1. The crossover aspects are more easily seen if we use the successive estimates $z_n(\eta)$ and $\tilde{z}_n(\eta)$ and $\tilde{z}_n(\eta)$ defined by (4.12) with X replaced by Δ and $\tilde{\Delta}$, respectively, and $g_c(\eta) = 1$.

Thus, for very large n we can expect $z_n(0) \to z_0$ and $z_n(\eta) \to z$ for $\eta > 0$, with analogous definitions for $\tilde{z}_n$. In figure 2 we plot $z_n(\eta)$ and $\tilde{z}_n(\eta)$ as functions of $1/n$, in which the crossover effects are apparent from the bending over of the curves with $\eta = 0.2$ and 0.4 as n increases.

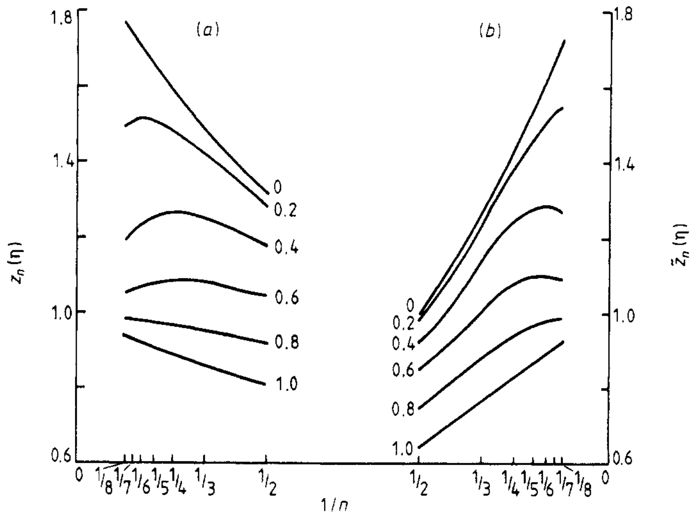

Figure 2. Asymptotic behaviour of the estimates for the dynamic exponents associated with the gaps in figure 1. The curves are labelled by the anisotropy η.

Although the asymptotic behaviour is independent of the boundary conditions imposed, previous calculations on the transverse Ising model (dos Santos 1980) indicate that FSS estimates converge faster to the exact results when periodic conditions (PBC) are imposed than for a system with free ends. In the case of the TXYM [1], however, for the chain with PBC the ground state is degenerate at ($g = 1$, $\eta = 0$) *for all n*, as opposed to the free ends case where this degeneracy builds up only asymptotically. The degeneracy in the ground state actually occurs along the unit circle $g^2 + \eta^2 = 1$ for any finite size transverse XY chain with PBC. Since in this case the states can be classified according to a wavevector k, the ground state ($k = 0$ mode) must transform according to the $k = 0$ mode of an operator which is a symmetry operation only for $g^2 + \eta^2 = 1$. For this reason we will refer to this degeneracy as 'accidental'. Therefore, $\Delta_n(1, 0) \equiv 0$ so that we cannot detect $z_n(0) \to 2$ as $n \to \infty$ as before. This fact is illustrated in figure 3(a) where the curve corresponding to $\eta = 0.1$ has a small slope, whereas figure 3(b), corresponding to $\tilde{\Delta}$, displays the same behaviour as for the chain with free ends. Again, the crossover effects are more pronounced by the bending over of the curves in figure 4.

The results of the calculations with the energy gaps can then be summarised as follows (if one regards the behaviour of Δ_n for the chain with PBC as $\eta \to 0$ as being 'accidental').

(i) $$\lim_{n\to\infty} z_n(\eta) = \lim_{n\to\infty} \tilde{z}_n(\eta). \qquad (5.6)$$

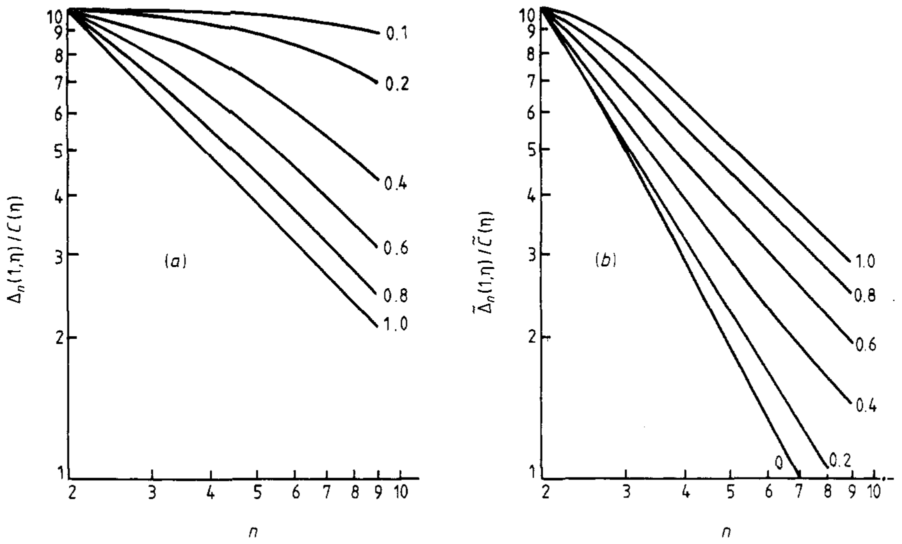

Figure 3. Normalised energy gaps between the ground state and both the first (a) and the second (b) excited states as functions of n at constant anisotropy, for chains with periodic boundary conditions. The curves are labelled by the values of η.

(ii) $$\lim_{n\to\infty} z_n(\eta) = \begin{cases} 1 & \text{if } \eta > 0, \\ 2 & \text{if } \eta = 0. \end{cases} \tag{5.7}$$

The equality between the exponent relative to the gaps Δ and $\tilde{\Delta}$ reflected by (5.6), to our knowledge, had never been established, but the results for z agree with previous exact calculations for $0 < \eta \leq 1$ (Pfeuty 1970, Suzuki 1971, Barouch and McCoy 1971, Young 1975) and with RG calculations (Gerber and Beck 1977, Jullien and Pfeuty 1979) for $\eta = 0$.

5.2. Longitudinal susceptibilities χ^{xx} and χ^{yy}

The behaviour of the susceptibilities along the x and y directions in spin space should be quite analogous to that of the two correlation lengths discussed in § 3. Indeed, for $\eta = 0$ the roles of σ^x and σ^y can be interchanged and thus $\chi^{xx} = \chi^{yy}$. For any finite amount of positive anisotropy, however, the yy coupling becomes irrelevant (in the RG sense) so that χ^{yy} should not diverge at $g_c(\eta)$, whereas χ^{xx} should diverge with the same exponent as for the transverse Ising model. Analogously, for $\eta < 0$ χ^{yy} should diverge but not χ^{xx}.

If one includes a field in the xy plane, one should add

$$H_{\text{field}} = -h^x \sum_i \sigma_i^x - h^y \sum_i \sigma_i^y \tag{5.8}$$

to the Hamiltonian (5.1), so that at zero temperature the zero field susceptibilities for a system of N spins are defined by

$$\chi^{\mu\mu}(g, \eta) = -\frac{1}{N}\left(\frac{\partial^2 E_0(g, \eta, h^x, h^y)}{\partial h^{\mu 2}}\right)_{h^x = h^y = 0} \tag{5.9}$$

where $\mu = x, y$, and $E_0(g, \eta, h^x, h^y)$ is the ground state energy. In the thermodynamic

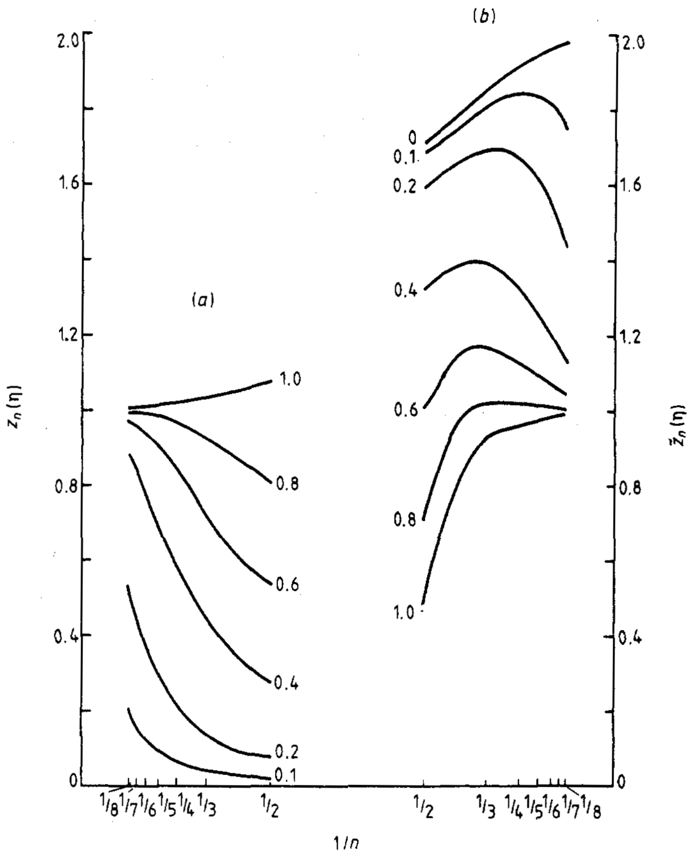

Figure 4. Asymptotic behaviour of the estimates for the dynamic exponents associated with the gaps in figure 3. The curves are labelled by the anisotropy η.

limit we then expect for g near $g_c(\eta)$, $\eta \geqslant 0$,

$$\chi^{xx}(g, 0) = \chi^{yy}(g, 0) \sim |g - g_c(0)|^{-\gamma_0}, \tag{5.10}$$

$$\chi^{xx}(g, \eta) \sim |g - g_c(\eta)|^{-\gamma}, \tag{5.11}$$

$$\chi^{yy}(g, \eta) \sim \Phi(g, \eta), \tag{5.12}$$

where Φ is a smooth and well behaved function of $\eta > 0$. This means that for a system of finite (but large) size n the EFSS hypothesis yields

$$\chi_n^{xx}(1, 0) = \chi_n^{yy}(1, 0) \approx n^{\gamma_0/\nu_0} \tag{5.13}$$

for $\eta = 0$, and

$$\chi_n^{xx}(1, n) \approx n^{\gamma/\nu} f_1(\eta) \tag{5.14}$$

and

$$\chi_n^{yy}(1, \eta) \approx n^{\tilde{\gamma}/\nu} \tilde{f}_2(\eta) \tag{5.25}$$

for $\eta > 0$. Note that the absence of power law singularity in the thermodynamic limit is reflected by n independence in the FSS hypothesis, so we expect $\tilde{\gamma} = 0$.

Contrary to what happens for the energy gaps, the difference between the two limiting slopes of a log–log plot of χ^{xx} against n is not easily noticed: $\gamma/\nu = 1.75$ (Pfeuty 1970) and $\gamma_0/\nu_0 = 2$ (Gerber and Beck 1977). Thus, instead of a log–log plot of χ^{xx} against n, we show in figure 5 the successive estimates $\psi_n(\eta)$ as defined by (4.12) for a chain with free ends. Following equations (4.13) and (4.14), we then expect

$$\psi_n(\eta) \underset{n\to\infty}{\to} \begin{cases} \gamma/\nu & \text{if } \eta \neq 0, \\ \gamma_0/\nu_0 & \text{if } \eta = 0. \end{cases} \tag{5.16}$$

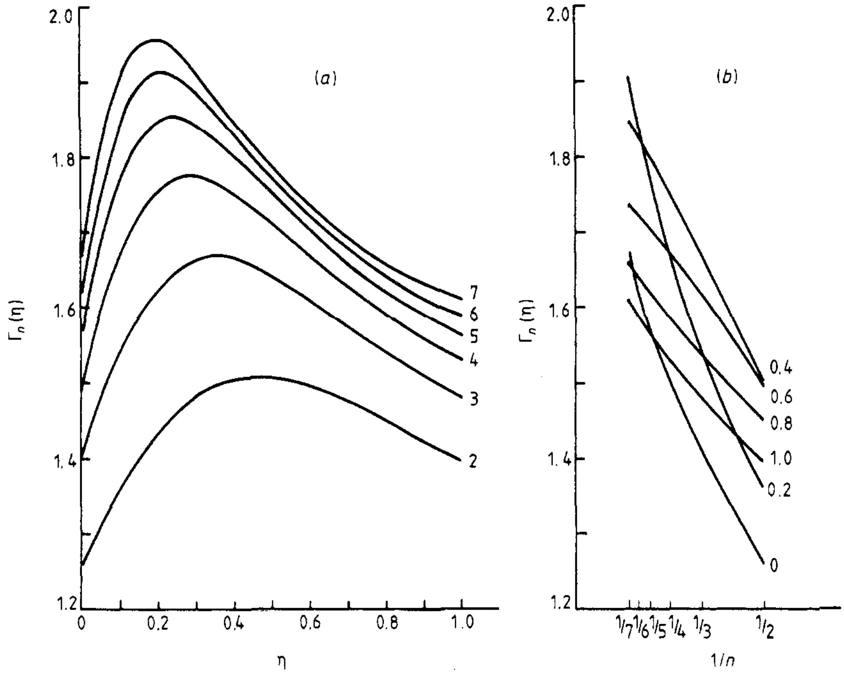

Figure 5. (a) Successive estimates of the ratio between the XX susceptibility and correlation length exponents as functions of η, for chains with free ends, obtained from equation (4.12) with $X \equiv \chi^{xx}$ and $\psi_n \equiv \Gamma_n$. The curves are labelled by n. (b) Asymptotic behaviour of these estimates for different values of the anisotropy η which labels the curves.

Indeed, in figure 5(a) the height and position of the maximum of $\psi_n(\eta)$ seem to be converging towards the values 2 and 0, respectively. Figure 5(b) displays the behaviour of these estimates as functions of $1/n$. Unfortunately, the sizes of the systems accessible numerically are not large enough to verify the bending over found for the gaps.

The results for χ^{yy} are shown in figure 6. We note from figure 6(a) that as η increases from zero the curves tend to flatten down for large n, indicating the absence of power law singularity. As a guide to the limiting n behaviour, figure 6(b) shows successive estimates of $\tilde{\gamma}/\nu$ as functions of $1/n$, where the bending over towards the value zero is already apparent from the curve corresponding to $\eta = 0.1$.

For a chain with periodic boundary conditions, the effects of degeneracy are felt in the susceptibility as well. The calculations performed in this case indicate that χ^{xx} and χ^{yy} diverge even for a finite system as $\eta \to 0$, although $\lim_{\eta\to 0}[\chi^{\mu\mu}_{n+1}(1,\eta)/\chi^{\mu\mu}_n(1,\eta)] = 1$. Again all information about the isotropic limit is

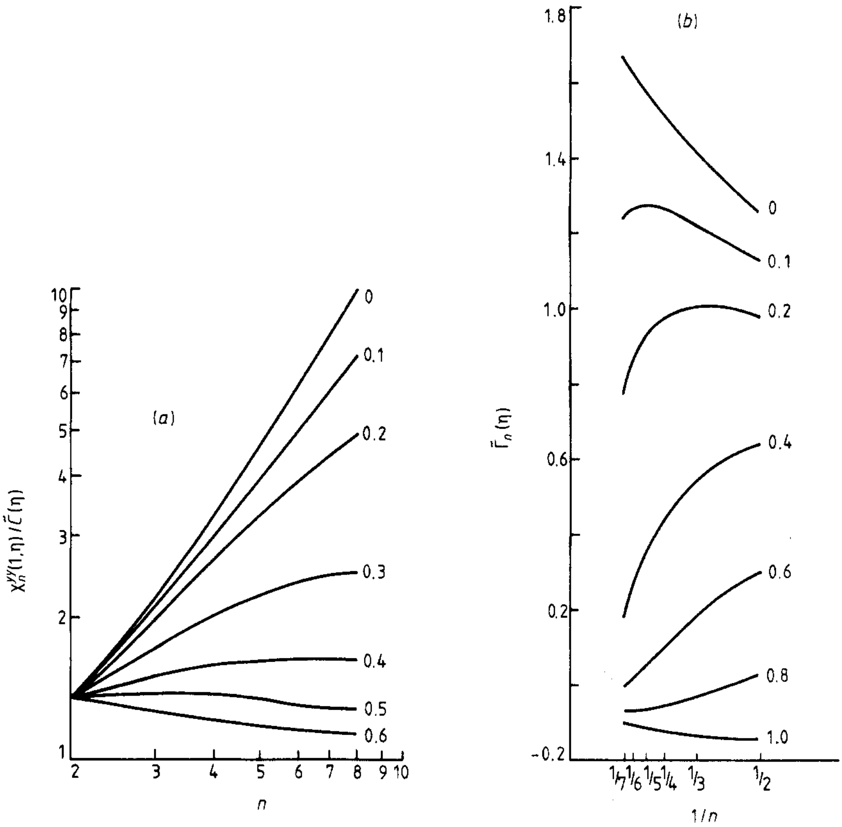

Figure 6. (*a*) Normalised *YY*-susceptibility as a function of n at constant anisotropy η, for chains with free ends. The curves are labelled by the values of η. (*b*) Asymptotic behaviour of the corresponding slopes, according to equation (4.12) with $X \equiv \chi^{yy}$ and $\psi_n(\eta) \equiv \tilde{\Gamma}_n(\eta)$.

lost because of this behaviour. Even so, one can detect a change in the behaviour as η is increased from 0, as shown in figures 7(*a*) and 7(*b*). In particular, we note from figure 7(*a*) that the curves corresponding to $\eta = 0.6$, 0.8 and 1, respectively, are nearly parallel in the largest n region considered. Actual numbers for successive slopes can be extracted from figure 7(*b*), where the trend indicates quite neatly that all curves with $\eta \geq 0.2$ tend to a common limit around 1.75, the exact result.

The results for χ^{yy} for a chain with periodic boundary conditions are displayed in figure 8(*a*), from which we notice the flattening down of the curve corresponding to $\eta \geq 0.4$, in agreement with the free ends case. The behaviour is also apparent from figure 8(*b*), where after an initial non-zero value for $\tilde{\gamma}$, the values tend to zero as η increases.

Thus, if one again neglects the behaviour at $\eta = 0$ for a chain with PBC, the results for the susceptibility can be summarised as follows:

(i) $$\lim_{n\to\infty} (\gamma_0/\nu_0)_n = \lim_{n\to\infty} (\tilde{\gamma}_0/\nu_0)_n = 2,$$

(ii) $$\lim_{n\to\infty} (\gamma/\nu)_n = 1.75,$$

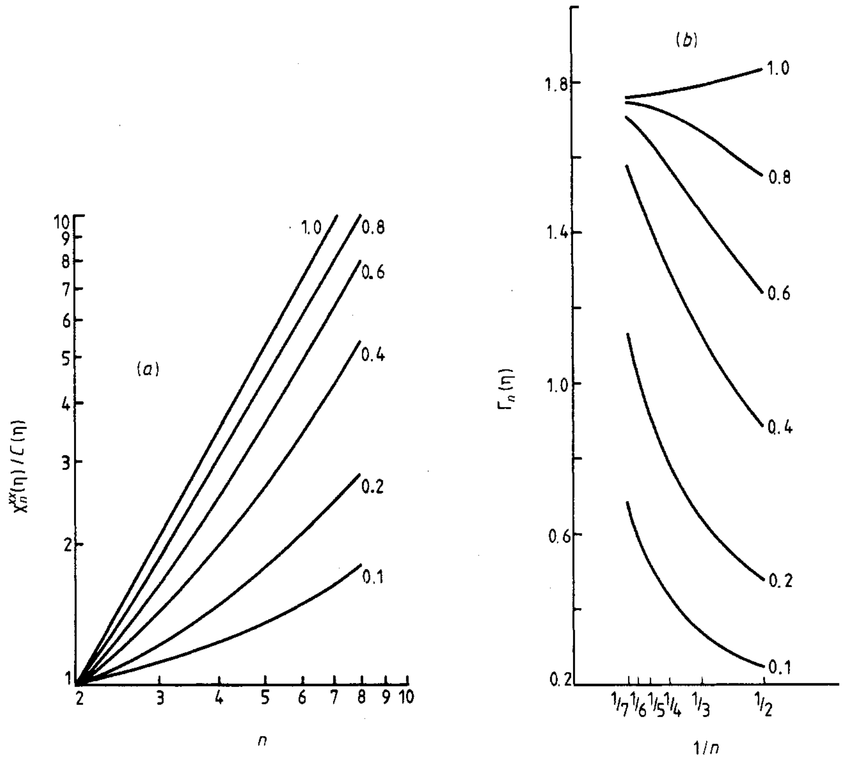

Figure 7. (a) Normalised XX-susceptibility as a function of n at a constant anisotropy η, for chains with periodic boundary conditions. The curves are labelled by the values of η. (b) Asymptotic behaviour of the corresponding slopes, according to equation (4.12), with $X \equiv \chi^{xx}$ and $\psi_n(\eta) \equiv \Gamma_n(\eta)$.

(iii) $$\lim_{n\to\infty} (\tilde{\gamma}/\nu)_n = 0,$$

where we have extended the notation from equation (5.16). This picture agrees with the exact results for γ, ν and ν_0 (Pfeuty 1970, Barouch and McCoy 1971), and with approximate results for γ_0 (Gerber and Beck 1977).

As mentioned in § 4, the ratio ϕ/ν_0 can be estimated in the same way as we calculated x/ν_0, but with X_n replaced by its logarithmic derivative. As the energy levels are even functions of η (due to the symmetry of the Hamiltonian), we have to use the susceptibility to calculate ϕ/ν_0, the results of which are shown in table 1.

As $\nu_0 = \frac{1}{2}$, and the above results seem to indicate that $\lim_{n\to\infty} (\phi/\nu_0) = 1$, we obtain $\phi = \frac{1}{2}$. This is consistent with the conclusions of a careful analysis (to be published) of the results of Barouch and McCoy (1971).

As a final test of these ideas we show in figure 9 log–log plots both of $n\Delta_n(g = 1, \eta)$ and of $n^{-1.75}\chi_n^{xx}(g = 1, \eta)$ as functions of η. As expected, for small η the curves do not superpose, but for $\eta > 0.4$ the universal character is quite apparent. Moreover, from the behaviour near $\eta = 1$ we infer that the η dependence is given by a power law

$$n^{-x/\nu} X_n(1, \eta) \sim \eta^{\lambda}. \qquad (5.17)$$

Calculations with Δ_9 yield $\lambda = 1.02$, whereas calculations with χ_8 yield $\lambda = -0.76$.

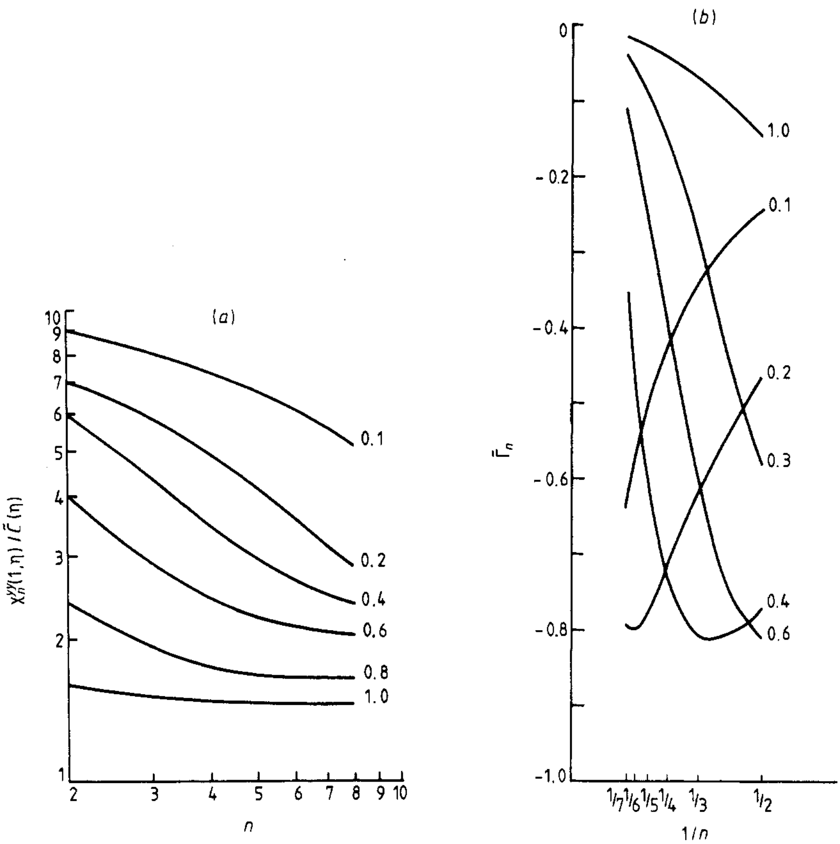

Figure 8. (*a*) Normalised *YY*-susceptibility a a function of n at constant anisotropy η, for chains with periodic boundary conditions. The curves are labelled by the value of η. (*b*) Asymptotic behaviour of the corresponding slopes, according to equation (4.12), with $X \equiv \chi^{yy}$ and $\psi_n(\eta) \equiv \tilde{\Gamma}_n(\eta)$.

Table 1. Successive estimates $(\phi/\nu_0)_n = \ln[\Psi_n(1)/\Psi_{n-1}(1)]/\ln(n/n-1)$ where $\Psi_n(1) = \{\partial/\partial\eta \ln \chi_n[g_c(\eta)]_{\eta=0}\}$ for the chain with free ends.

n	$(\phi/\nu_0)_n$
6	1.20
7	1.14
8	1.13

6. Discussion and conclusion

The extension of the FSS hypothesis (Fisher 1971) to treat crossover phenomena was achieved with the introduction of a second scaling variable, the choice of which was dictated by requiring certain consistency conditions to be satisfied, as discussed in § 4. As the set of scaling variables should reflect the competition between two distinct critical behaviours, one could, in principle, use the ratio between the two correlation

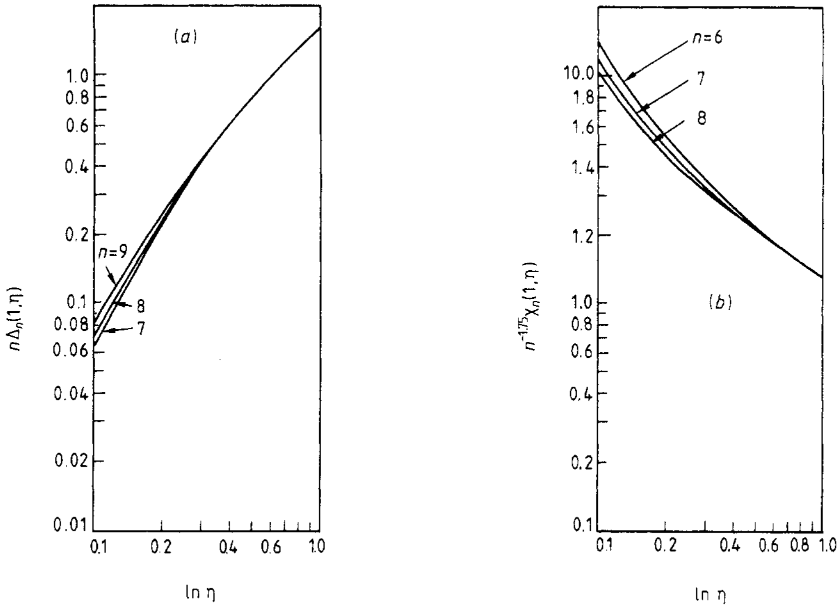

Figure 9. Universal plots of the scaled energy gap Δ_n (a) and scaled XX-susceptibility χ_n^{xx} (b) as in equation (4.10), as functions of η, for chains with periodic boundary conditions. The curves are labelled by the size of the chains.

lengths. This possibility, however, would not allow us to modify the n exponent, which would imply $x_0/\nu_0 = x/\nu$ which is not always true. Another comment with respect to the choice of scaling variables concerns the actual rounding of the critical line. As mentioned in § 2 in connection with the usual FSS hypothesis, the inhibition of the critical behaviour relative to the infinite system is due to the correlation length being of the order of the size of the system. In this sense one could scale (Fisher 1971) with the correlation length being measured from the distance to a critical or pseudo-critical line (if the system is infinite in one or more dimensions, or if it is totally finite, respectively). The extension to crossover phenomena can follow along the same lines, by defining a critical (or pseudo-critical) line $g_c(n;\eta)$.

As a final comment, we note that FSS is limited by its inability to calculate all critical properties of interest. Firstly, the critical point (or critical curve) must be given rather accurately. Secondly, the information about critical exponents that we obtain is always as a ratio between the exponent associated with the quantity used and the correlation length exponent. In principle, one could overcome the first limitation by using a quantity with a rounded off singularity for systems of finite size. That is, instead of being a monotonic function it displays maxima along a pseudo-critical line $g_c(n;\eta)$ which, for large n, should be a reasonable estimate $\tilde{g}_c(\eta)$ for the limiting curve $g_c(\eta)$. We could then use $\tilde{g}_c(\eta)$ to obtain the exponent ratios as outlined at the end of § 4. We can overcome the second limitation if we obtain FSS estimates from two quantities with exponents linked by a scaling law. We could then have an extra equation, so that each exponent could be calculated independently.

Away from the crossover region, there is another way of overcoming these difficulties which is the so-called finite size rescaling transformation (dos Santos and Sneddon 1981). Within this scheme, which is close in spirit to the usual renormalisation group, a fixed point of the transformation is found, and linearisation around it yields the correlation length exponent. With the aid of the EFSS hypothesis we can now pursue ways of removing the restriction concerning the validity of the finite size rescaling transformation around the crossover region.

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