Critical behaviour of semi-infinite systems

1977 J. Phys. A: Math. Gen. 10 1927

(http://iopscience.iop.org/0305-4470/10/11/021)

J. Phys. A: Math. Gen., Vol. 10, No. 11, 1977. Printed in Great Britain. © 1977

Critical behaviour of semi-infinite systems

A J Bray and M A Moore
Department of Theoretical Physics, The University, Manchester, M13 9PL, UK

Received 20 April 1977

Abstract. The critical behaviour of a semi-infinite system with O(n) spin symmetry is investigated using four techniques: (i) mean-field theory, (ii) exact solution for $n=\infty$, (iii) the ϵ expansion, and (iv) scaling arguments. The surface equation of state is computed using mean-field theory, and the four phase transitions defined by Lubensky and Rubin, the 'ordinary', 'surface', 'extraordinary', and '$\lambda=\infty$' ('special') transitions, are identified. The first three may be observed in the bulk system by adding a suitable 'surface' perturbation which destroys translational invariance. Scaling arguments give their critical exponents exactly in terms of bulk exponents. Critical exponents for the '$\lambda=\infty$' transition are determined for $n=\infty$ and also to O(ϵ). Spin–spin correlation functions at $T=T_c$ for the 'ordinary', 'extraordinary' and '$\lambda=\infty$' transitions are calculated exactly for $n=\infty$.

1. Introduction

The effects of surfaces on phase transitions have received a great deal of attention in recent years. Techniques developed for the study of phase transitions in bulk systems have been applied to systems with surfaces, with varying degrees of success. Such techniques include mean-field theories (Mills 1971, Kaganov and Omelyanchouk 1971, Béal-Monod *et al* 1972, Weiner *et al* 1973, Wolfram *et al* 1971, Binder and Hohenberg 1972, 1974, Lubensky and Rubin 1975a), high-temperature series expansions (Binder and Hohenberg 1972, 1974), low-temperature series expansions (Barber 1973a, b), Monte Carlo analyses (Binder and Hohenberg 1974, Binder 1972), scaling analyses (Binder and Hohenberg 1972, 1974, Barber 1973a, Fisher 1971, 1973), ϵ expansions (Lubensky and Rubin 1973, 1975b), exact solutions for the two-dimensional Ising model (McCoy and Wu 1967, Fisher and Ferdinand 1967, Ferdinand and Fisher 1969, Au-Yang 1973) and exact solutions for two spherical models (Fisher and Barber 1972, 1973, Barber 1974, Barber *et al* 1974, Singh *et al* 1975).

It has recently become apparent that the theory of phase transitions in semi-infinite systems is much richer than had hitherto been supposed. Using a mean-field theory analysis, Lubensky and Rubin (1975a, to be referred to as LR) have identified four separate phase transitions associated with the surface. They call these the 'ordinary', 'surface', 'extraordinary' and '$\lambda=\infty$' transitions though we shall see later that this nomenclature is not entirely satisfactory. We review the LR classifications scheme here. The phase transition is modelled by the usual Ginzburg–Landau–Wilson Hamiltonian for a system with O(n) spin symmetry, containing an extra 'surface' contribution:

$$H=\int \mathrm{d}^d x\Big[\tfrac{1}{2}t\sum_{i=1}^{n}\phi_i^2(\boldsymbol{x})+\tfrac{1}{2}\sum_{i=1}^{n}(\nabla\phi_i)^2+\frac{u}{4}\Big(\sum_{i=1}^{n}\phi_i^2(\boldsymbol{x})\Big)^2$$
$$+\tfrac{1}{2}c\delta(z)\sum_{i=1}^{n}\phi_i^2(\boldsymbol{x})-h_1\delta(z)\phi_1(\boldsymbol{x})\Big]. \tag{1.1}$$

Here $\phi_i(\boldsymbol{x})$ is the ith Cartesian component of the n-component order parameter, and $t\propto(T-T_c^{MF})$ where T_c^{MF} is the mean-field transition temperature. The integration over $\boldsymbol{x}$ in equation (1.1) is over the half-space $z\geqslant 0$. The term in c is a surface perturbation which changes locally the value of T_c^{MF}. For a spin model on a lattice, with nearest-neighbour exchange interaction $J(1+\Delta)$ between spins in the surface layer, and exchange interaction J between all other nearest-neighbour pairs of spins, it may be shown that (Mills 1971, Binder and Hohenberg 1972, 1974, LR)

$$c=[1-2(d-1)\Delta]/a \tag{1.2}$$

where d is the dimensionality of the system and a is the lattice spacing. In mean-field theory, the spontaneous magnetisation $\langle\phi_1(z)\rangle$ is linear in z for small z and extrapolates to zero at $z=-c^{-1}$. Therefore c^{-1} is called the 'extrapolation length' in the literature and is usually denoted by the symbol λ.

The field h_1 in equation (1.1) acts only in the surface and is parallel to the '1' direction in spin space. A uniform field would produce an extra term in the Hamiltonian, but we omit this for simplicity.

The types of phase transition which are possible with the Hamiltonian (1.1) have been classified by LR using mean-field theory. For $c>0$ the system orders at the bulk transition temperature T_c. This is the 'ordinary' transition. For $c<0$ the mean-field transition temperature in the surface exceeds that in the bulk, and the surface orders spontaneously at a higher temperature than the bulk. This is the 'surface' transition. As the temperature is lowered through the bulk critical temperature in the presence of the ordered surface, there is a second phase transition as the bulk orders. LR term this the 'extraordinary' transition. Finally, the case $c=0$ corresponds to an enhanced exchange interaction between surface spins (see equation (1.2)) which is not quite strong enough to split off a surface phase. For this case the system orders at the bulk transition temperature, but the critical exponents and correlation functions differ from those of the 'ordinary' transition. LR call this the '$\lambda=\infty$' transition (recall $\lambda=c^{-1}$). This terminology is a little unfortunate, however, since the concept of an extrapolation length has no validity outside mean-field theory (Binder and Hohenberg 1972). The '$\lambda=\infty$' transition is associated with that value of c such that the enhanced surface exchange is not quite sufficient to split off a surface phase, and in general this critical value of c will be different from zero. For example, the work of Binder and Hohenberg (1974) on the semi-infinite three-dimensional Ising model indicates that the existence of a surface phase requires $\Delta>\Delta_c\simeq 0{\cdot}6$, compared to the mean-field value $\Delta_c=1/4$. Equation (1.2) then gives the value of c appropriate to the '$\lambda=\infty$' transition as $c^*\sim -1{\cdot}4/a$. To avoid confusion we will use the term 'special transition' to describe the phase transition associated with this critical value of c.

Of the four transitions described above, the ordinary and surface transitions (especially the former) have received by far the most attention in the literature, results for the extraordinary and special transitions being restricted to mean-field theory (LR). In the present paper we investigate all four transitions using a variety of techniques:

mean-field theory, exact solution at $T = T_c$ for the case $n = \infty$, expansion in powers of $\epsilon = 4 - d$, and scaling analyses. Mean-field theory is used to compute the surface equation of state, to exemplify all four transitions, and to introduce the thermodynamic critical exponents. These will be labelled with subscripts '1' (to indicate that they are surface exponents) and superscripts s, e, sp corresponding to the surface, extraordinary and special transitions respectively. Exponents for the ordinary transition will carry no superscripts, in accordance with standard convention. In the limit $n \to \infty$, spin–spin correlation functions at $T = T_c$ for the ordinary, extraordinary and special transitions may be computed exactly, and determine the correlation exponents in this limit.

Perhaps the most significant result of the paper is the observation that the ordinary, surface and extraordinary transitions may all be observed in the bulk system, i.e. the system for which the integration in equation (1.1) extends over all space, because the terms in c and h_1 break the translational invariance in the same way as a true surface. This observation enables us to use scaling arguments to determine *exactly* the critical exponents for these transitions in terms of the standard bulk exponents α, β, γ, δ, η, ν, Δ, etc. For the infinite (i.e. bulk) system, however, the critical value of c for splitting off a surface phase is $c^* = 0$: the 'surface' (i.e. the plane $z = 0$) orders at a higher temperature than the bulk for any $c < 0$, provided that the $(d-1)$-dimensional system can order spontaneously at finite temperature. Hence for the infinite system the special transition is replaced by the bulk transition, and we are therefore unable to determine the exponents of the special transition by means of scaling arguments.

The paper is organised according to computational technique. Thus § 2 is devoted to mean-field theory, § 3 to the large n limit, § 4 to the ϵ expansion, and § 5 to scaling arguments. Sections 6 and 7 contain a discussion and summary of the results respectively.

2. Mean-field theory: surface equation of state

Mean-field theory has been applied to the semi-infinite problem by several authors (see § 1). Although the techniques used here are, therefore, not new, a mean-field description serves to exemplify explicitly the four types of transition. In addition, our identifications of the critical exponents, particularly for the extraordinary transition, differ from those conventionally made, but are consistent with the scaling arguments of § 5. A discussion of mean-field theory is therefore not without interest.

The mean-field approach consists of minimising the Hamiltonian H of equation (1.1) with respect to the vector order parameter $\boldsymbol{\phi}(\boldsymbol{x}) = (\phi_1, \ldots, \phi_n)$. The vector $\boldsymbol{\phi}(\boldsymbol{x})$ which minimises H will be parallel to the surface field h_1 and, because of translational invariance parallel to the surface, will depend only on the distance z from the surface. Denoting its absolute value by $m(z)$ we find (LR)

$$m''(z) = tm(z) + um^3(z), \qquad z > 0 \tag{2.1}$$

$$m'(0) = cm(0) - h_1 \tag{2.2}$$

where primes indicate derivatives with respect to z. Equation (2.1) may easily be integrated once, by multiplying through by $m'(z)$, to give

$$(m'(z))^2 = tm^2(z) + \tfrac{1}{2}um^4(z) + C \tag{2.3}$$

where C is a constant of integration. For $t>0$ the magnetisation density $m(z)$ decays to zero in the bulk, i.e. $m'(z)<0$ and $m(\infty)=0=m'(\infty)$. Therefore we choose $C=0$ in equation (2.3) and take the negative square root to give

$$m'(z)=-m(z)(t+\tfrac{1}{2}um^2(z))^{1/2}. \tag{2.4}$$

Using the boundary condition (2.2), and writing $m(0)=m_1$, we obtain the equation of state for the surface:

$$h_1=m_1[c+(t+\tfrac{1}{2}um_1^2)^{1/2}], \qquad t>0. \tag{2.5}$$

For $t<0$, the magnetisation density $m(z)$ decays to the bulk value $(-t/u)^{1/2}$ as $z\to\infty$. Therefore, we choose $C=t^2/2u$ in equation (2.3) so that we recover the bulk results $m'(\infty)=0$, $m(\infty)=(-t/u)^{1/2}$. Since $m'(z)$ has the same sign as $|t|-um^2$ ($m'<0$ if $m(z)>m(\infty)$ and *vice versa*), we take the negative square root in equation (2.3) to give

$$m'(z)=-(\tfrac{1}{2}u)^{1/2}(m^2(z)-|t|/u). \tag{2.6}$$

Using the boundary condition (2.2) we obtain the surface equation of state for $t<0$:

$$h_1=cm_1+\frac{1}{(2u)^{1/2}}(um_1^2-|t|), \qquad t<0. \tag{2.7}$$

2.1. *The ordinary transition*

This corresponds to the case $c>0$, and the limit $h_1\to 0$. Equations (2.5) and (2.7) may be simplified by introducing the scaled variables

$$\tilde{h}=(\tfrac{1}{2}u)^{1/2}\frac{h_1}{c^2}, \qquad \tilde{m}=(\tfrac{1}{2}u)^{1/2}\frac{m_1}{c}, \qquad \tilde{t}=\frac{t}{c^2}$$

giving

$$\tilde{h}=\tilde{m}[1+(\tilde{t}+\tilde{m}^2)^{1/2}], \qquad \tilde{t}>0 \tag{2.8a}$$

$$\tilde{h}=\tilde{m}+\tilde{m}^2-\tfrac{1}{2}|\tilde{t}|, \qquad \tilde{t}<0. \tag{2.8b}$$

The local susceptibility $\chi_{1,1}$ gives the response of a spin in the surface to a magnetic field applied in the surface. Its singular part behaves as $t^{-\gamma_{1,1}}$ as $t\to 0$, defining the critical exponent $\gamma_{1,1}$. In scaled variables we have, for $\tilde{t}>0$,

$$\tilde{\chi}_{1,1}\equiv\frac{\mathrm{d}\tilde{m}}{\mathrm{d}\tilde{h}}\bigg|_{\tilde{h}=0}=(1+\tilde{t}^{1/2})^{-1}=1-\tilde{t}^{1/2}+\mathrm{O}(\tilde{t}) \tag{2.9}$$

giving

$$\gamma_{1,1}=-\tfrac{1}{2}. \tag{2.10}$$

The spontaneous surface magnetisation varies as $|\tilde{t}|^{\beta_1}$ as $\tilde{t}\to 0-$. Setting $\tilde{h}=0$ in equation (2.8*b*) yields

$$\tilde{m}=\tfrac{1}{2}|\tilde{t}|+\mathrm{O}(\tilde{t}^2) \tag{2.11}$$

giving

$$\beta_1=1. \tag{2.12}$$

For $\tilde{t}=0$, both equations (2.8*a*) and (2.8*b*) reduce to

$$\tilde{h}=\tilde{m}+\tilde{m}^2 \tag{2.13}$$

or

$$\tilde{m}=\tilde{h}-\tilde{h}^2+\mathrm{O}(\tilde{h}^3). \tag{2.14}$$

Now we come to a subtle point. The critical exponent $\delta_{1,1}$ would normally be defined, by analogy with the bulk definition, by the relation $\tilde{m}\propto\tilde{h}^{1/\delta_{1,1}}$ as $\tilde{h}\to 0$. According to equation (2.14), this definition gives $\delta_{1,1}=1$. However, this is somewhat misleading for the present case in which $\gamma_{1,1}<0$ implies that the susceptibility $\tilde{\chi}_{1,1}$ is finite at $\tilde{t}=0$ as shown explicitly in equation (2.9). For such a case $\tilde{m}$ is always proportional to $\tilde{h}$ for small $\tilde{h}$. It makes sense, therefore, to disregard this 'regular' contribution to $\tilde{m}$ in computing $\delta_{1,1}$, just as the '1' in equation (2.9) was disregarded in computing $\gamma_{1,1}$. The value of $\delta_{1,1}$ is then determined from the second term on the right-hand side of equation (2.14), namely

$$\delta_{1,1}=\tfrac{1}{2}. \tag{2.15}$$

All this becomes clearer when we try to write the equation of state in canonical scaling form:

$$\tilde{m}=\tilde{t}^{\beta_1}f(\tilde{h}/\tilde{t}^{\Delta_1}) \tag{2.16}$$

where the function f has different forms according to the sign of $\tilde{t}$, and Δ_1 is the 'surface gap exponent'. From equation (2.16) one immediately derives the scaling laws

$$-\gamma_{1,1}=\beta_1-\Delta_1 \tag{2.17a}$$

$$\delta_{1,1}=\Delta_1/\beta_1. \tag{2.17b}$$

Elimination of Δ_1 yields a relation between β_1, $\gamma_{1,1}$ and $\delta_{1,1}$:

$$\gamma_{1,1}=\beta_1(\delta_{1,1}-1) \tag{2.18}$$

which is satisfied by the exponent values given in equations (2.10), (2.12) and (2.15). Our definition of $\delta_{1,1}$ is motivated by a desire to preserve the validity of such scaling laws. Equations (2.8) can be written in the form of equation (2.16) if one first subtracts from $\tilde{m}$ the regular contribution $\tilde{h}$. The difference $\hat{m}$ satisfies, in the scaling regime $\tilde{m}\ll 1$, $\tilde{h}\ll 1$, $\tilde{t}\ll 1$ the equations

$$\hat{m}=\tilde{m}-\tilde{h}=-\tilde{t}[1+(\tilde{h}^2/\tilde{t})]^{1/2}, \qquad \tilde{t}>0 \tag{2.19a}$$

$$\hat{m}=\tilde{m}-\tilde{h}=\tfrac{1}{2}|\tilde{t}|[1-(2\tilde{h}^2/|\tilde{t}|)], \qquad \tilde{t}<0 \tag{2.19b}$$

which have the form of equation (2.16) and from which one identifies

$$\Delta_1=\tfrac{1}{2} \tag{2.20}$$

satisfying the scaling laws, equations (2.17). We have stressed these points rather strongly in order to emphasise that, in a case where the susceptibility is finite at the critical point, the critical exponents must be identified very carefully in order to preserve the scaling laws. This point will reappear in the discussion of the extraordinary transition.

2.2 *The surface transition*

This corresponds to the case $c<0$ and the limit $h_1 \to 0$. Introducing the scaled variables

$$\tilde{h} = (\tfrac{1}{2}u)^{1/2}\frac{h_1}{|c|^2}, \qquad \tilde{m} = (\tfrac{1}{2}u)^{1/2}\frac{m_1}{|c|}, \qquad \tilde{t} = \frac{t}{|c|^2}$$

in equations (2.5) and (2.7) yields the equation of state:

$$\tilde{h} = \tilde{m}[(\tilde{t}+\tilde{m}^2)^{1/2}-1], \qquad \tilde{t}>0 \tag{2.21a}$$

$$\tilde{h} = \tilde{m}^2 - \tilde{m} - \tfrac{1}{2}|\tilde{t}|, \qquad \tilde{t}<0. \tag{2.21b}$$

In zero field the magnetisation may be computed in closed form:

$$\tilde{m} = 0, \qquad \tilde{t}>1 \tag{2.22a}$$

$$\tilde{m} = (1-\tilde{t})^{1/2}, \qquad 1>\tilde{t}>0 \tag{2.22b}$$

$$\tilde{m} = \tfrac{1}{2}+\tfrac{1}{2}(1+2|\tilde{t}|)^{1/2}, \qquad \tilde{t}<0. \tag{2.22c}$$

The point $\tilde{t}=1$ gives the critical temperature for the surface transition. In terms of unscaled variables we have a critical temperature

$$t_c = |c|^2 \tag{2.23}$$

below which the surface orders spontaneously. We define the 'bulk-surface crossover exponent' ϕ_s by the relation

$$t_c \propto |c|^{1/\phi_s}, \qquad |c|\to 0 \tag{2.24}$$

from which we deduce

$$\phi_s = \tfrac{1}{2} \tag{2.25}$$

in mean-field theory. The thermodynamic exponents for the surface transition may be obtained by setting $\tilde{t} = 1+\tau$ in equation (2.21*a*) so that τ measures the deviation from the surface critical temperature. In the scaling regime $\tau \ll 1$, $\tilde{m} \ll 1$, $\tilde{h} \ll 1$ equation (2.21*a*) has the scaling form

$$\tilde{h} = \tfrac{1}{2}\tilde{m}(\tau+\tilde{m}^2) \tag{2.26}$$

from which one deduces the exponent values

$$\beta_1^s = \tfrac{1}{2} \tag{2.27a}$$

$$\gamma_{1,1}^s = 1 \tag{2.27b}$$

$$\delta_{1,1}^s = 3 \tag{2.27c}$$

$$\Delta_1^s = \tfrac{3}{2} \tag{2.27d}$$

which satisfy the scaling laws, equations (2.17). The reader will note that these exponents are identical to the mean-field exponents for a bulk system and that equation (2.26) has the same form as the mean-field equation of state in the bulk, provided $\tilde{h}$ is regarded for this purpose as a bulk field and $\gamma_{1,1}$ as the usual bulk susceptibility exponent. This result is not surprising as one may readily suppose that the exponents associated with the surface phase of a d-dimensional system are simply the bulk exponents for the $(d-1)$-dimensional system. This supposition is supported by a scaling argument in § 5. In mean-field theory, of course, the exponents are independent of dimensionality.

2.3. *The extraordinary transition*

In their pioneering work LR described the extraordinary transition as the onset of bulk order in the presence of *spontaneous* surface order, and therefore associated it with the case $c<0$. We shall see, however, that the extraordinary transition is, in fact, much more general than this. It is associated with the onset of bulk order in the presence of an ordered surface, *irrespective of how the surface order is achieved.* In particular, the surface may be ordered, for any value of c, by simply applying a finite surface field h_1. Then the extraordinary transition is the ordering of the bulk at $t=0$ with h_1 held fixed.

For the moment, however, let us consider the extraordinary transition as originally conceived by LR, namely the case $c<0$ in the limit $h_1 \to 0$. The spontaneous surface magnetisation $\tilde{m}$ in the neighbourhood of the bulk transition ($\tilde{t}=0$) is given exactly by equations (2.22b) and (2.22c). Expanding these to $O(\tilde{t}^2)$ yields

$$\tilde{m} = 1 - \tfrac{1}{2}\tilde{t} - \tfrac{1}{8}\tilde{t}^2 + O(\tilde{t}^3), \qquad \tilde{t}>0 \tag{2.28a}$$

$$\tilde{m} = 1 - \tfrac{1}{2}\tilde{t} - \tfrac{1}{4}\tilde{t}^2 + O(\tilde{t}^3), \qquad \tilde{t}<0. \tag{2.28b}$$

Thus the magnetisation and its first derivative are continuous at $\tilde{t}=0$. The leading singularity occurs at $O(\tilde{t}^2)$, i.e. $\tilde{m}$ has a discontinuity in its second derivative at $\tilde{t}=0$. Hence, we identify the surface magnetisation exponent as

$$\beta_1^{e} = 2. \tag{2.29}$$

Similarly one may compute the susceptibility $\tilde{\chi}_{1,1}$. For $\tilde{t}>0$, we write equation (2.21a) as

$$(\tilde{t} + \tilde{m}^2)^{1/2} = 1 + (\tilde{h}/\tilde{m})$$

giving

$$\tilde{m}^2 = 1 - \tilde{t} + [2\tilde{h}/(1-\tilde{t})^{1/2}] + O(\tilde{h}^2)$$

or

$$\tilde{\chi}_{1,1} = (1-\tilde{t})^{-1}, \qquad \tilde{t}>0. \tag{2.30}$$

For $\tilde{t}<0$, we may solve equation (2.21b) in closed form:

$$\tilde{m} = \tfrac{1}{2} + \tfrac{1}{2}(1 + 2|\tilde{t}| + 4\tilde{h})^{1/2} \tag{2.31}$$

giving

$$\tilde{\chi}_{1,1} = (1-2\tilde{t})^{-1/2}, \qquad \tilde{t}<0. \tag{2.32}$$

Equations (2.30) and (2.32) may be expanded to $O(\tilde{t}^2)$:

$$\tilde{\chi}_{1,1} = 1 + \tilde{t} + \tilde{t}^2 + O(\tilde{t}^3), \qquad \tilde{t}>0 \tag{2.33a}$$

$$\tilde{\chi}_{1,1} = 1 + \tilde{t} + \tfrac{3}{2}\tilde{t}^2 + O(\tilde{t}^3), \qquad \tilde{t}<0. \tag{2.33b}$$

The singularity in $\tilde{\chi}_{1,1}$ is, like that in $\tilde{m}$, a discontinuity in the second derivative. This leads to the identification

$$\gamma_{1,1}^{e} = -2. \tag{2.34}$$

The reader should note that these identifications of the exponent values differ from those made by LR who, on the basis of the linear terms in equations (2.28), identified $\beta_1^e = 1$ and, on the grounds that $\chi_{1,1}$ has regular series expansions above and below T_c, identified $\gamma_{1,1}^e = 0$. We believe that the present identifications are more useful since they preserve the scaling laws, a point which will be discussed further in § 5. The identification of exponents is, in any case, rather academic for the extraordinary transition since the singularities are so weak that they will be virtually impossible to observe experimentally.

For the case of a fixed surface field h_1, the extraordinary transition is observed for arbitrary c. To see this we return to our basic equations of state, (2.5) and (2.7), and consider the limit $t \to 0$ at fixed h_1. Expanding the square root in equation (2.5) yields

$$h_1 = cm_1 + (\tfrac{1}{2}u)^{1/2} m_1^2 + \frac{t}{(2u)^{1/2}} + O(t^2), \qquad t > 0 \tag{2.35}$$

whereas equation (2.7) reads

$$h_1 = cm_1 + (\tfrac{1}{2}u)^{1/2} m_1^2 + \frac{t}{(2u)^{1/2}}, \qquad t < 0 \tag{2.36}$$

exactly. To $O(t)$ these equations are identical, and therefore provide expansions for m_1 in powers of t in which the linear term is independent of the sign of t. As in the case $c < 0$, $h_1 \to 0$ discussed above, the linear term is a regular contribution to $m_1(t)$, and the singularity in $m_1(t)$ takes the form of a discontinuity in the second derivative. The identifications $\beta_1^e = 2$, $\gamma_{1,1}^e = -2$ are thus seen to be a consequence of m_1 being finite at $t = 0$, regardless of whether the ordering is spontaneous or the result of an applied surface field.

We conclude by noting that, in mean-field theory, the singularity in the surface magnetisation (and susceptibility) is identical to that in the bulk free energy, namely, a discontinuity in the second derivative. In § 5 we argue that this is a general result, valid outside mean-field theory, and hence that $\beta_1^e = 2 - \alpha = -\gamma_{1,1}^e$ where α is the bulk specific heat exponent.

2.4. The special transition

In mean-field theory this is the case $c = 0$. According to equation (2.23), any negative value of c suffices to order the surface spontaneously below a critical temperature $t_c = |c|^2$. Hence $c = 0$ is the critical value for splitting off a surface phase. The critical exponents are simply those of the bulk. Setting $c = 0$ in equations (2.5) and (2.7), these reduce immediately to scaling form (we set $u = 2$ for simplicity):

$$\frac{h_1}{t} = \frac{m_1}{t^{1/2}}\left(1 + \frac{m_1^2}{t}\right)^{1/2}, \qquad t > 0 \tag{2.37a}$$

$$\frac{h_1}{t} = \frac{m_1^2}{t}\left(1 + \frac{t}{2m_1^2}\right), \qquad t < 0 \tag{2.37b}$$

from which one identifies the exponent values

$$\gamma_{1,1}^{sp} = \tfrac{1}{2} \tag{2.38a}$$

$$\beta_1^{sp} = \tfrac{1}{2} \tag{2.38b}$$

$$\delta_{1,1}^{\mathrm{sp}} = 2 \tag{2.38c}$$

$$\Delta_1^{\mathrm{sp}} = 1 \tag{2.38d}$$

satisfying the scaling laws, equations (2.17). These are the mean-field exponents for a bulk system, where the field related exponents $\gamma_{1,1}$, $\delta_{1,1}$ and Δ_1 refer to a field applied in the plane $z = 0$ only. Thus mean-field theory does not distinguish between an infinite and a semi-infinite system, at least as far as critical exponents are concerned (the correlation functions do differ slightly, see § 3). The equivalence of the special and bulk transitions does not hold outside mean-field theory, however. For the infinite system, the critical value of c for splitting of a surface phase is always $c = 0$ (§ 5), corresponding to the bulk transition, whereas for the semi-infinite system the critical value of c, which in this case corresponds to the special transition, is expected to be different from zero in general (§ 4).

3. Exact results for $n = \infty$

Most of the recent advances in the theory of critical phenomena in bulk systems have been achieved by means of the renormalisation group approach. Excellent review articles on this technique have been written by Ma (1973a, b), Fisher (1974) and Wilson and Kogut (1974). In terms of explicit calculations, the most useful results have been achieved by means of the Wilson–Fisher ϵ expansion (Wilson and Fisher 1972, Wilson 1972), and the $1/n$ expansion (Abe 1972, 1973a, b, Abe and Hikami 1973, Hikami 1973, Ma 1973a, b, Ferrell and Scalapino 1972a, b, Brézin and Wallace 1973), where $\epsilon = 4 - d$ and n is the number of components of the order parameter (or 'spin dimensionality').

For surface problems the lack of complete translational invariance renders these techniques much more difficult to apply. A calculation to order ϵ of the critical exponents for the ordinary transition, and of the spin–spin correlation function at $T = T_c$, has been performed by Lubensky and Rubin (1973, 1975b) using the full renormalisation group approach. As for the $1/n$ expansion, the $n = \infty$ limit itself, which is trivial in the bulk, has only recently been solved (Bray and Moore 1977a) for the ordinary transition. The computational problems involved in finding $O(1/n)$ corrections seem totally intractable at this time. In this section we present exact calculations of spin–spin correlation functions for the ordinary, extraordinary and special transitions, in the limit $n = \infty$.

First, however, we should make a few remarks about the spherical model. This model was invented by Berlin and Kac (1952) as an approximation to the Ising model. It consists of an array of Ising spins σ_i for which the restriction $\sigma_i = \pm 1$ for all sites i is removed in favour of allowing the spins σ_i to be continuous variables with a Gaussian distribution such that $\langle \sigma_i^2 \rangle = 1$, subject to an overall constraint that the sums of the squares of all the spins be equal to the number of spins N, i.e. $\Sigma_{i=1}^{N} \sigma_i^2 = N$. A revival of interest in this rather unphysical model stems from Stanley's demonstration (Stanley 1968) that its partition function is identical to that of a generalised Heisenberg model, with n-dimensional spin vectors, in the limit $n \to \infty$. Since that time the expressions '$n = \infty$ limit' and 'spherical model' have often been used interchangeably in the literature.

Stanley's proof of the equivalence of the usual spherical model and the $n = \infty$ limit breaks down for the surface problem. Rather it seems likely that the $n = \infty$ limit for this case corresponds to a spherical model in which a spherical constraint is applied separately to each layer parallel to the surface. Indeed, the first terms in a high-temperature series indicate that the system with $n=\infty$ and the system with constraints on each layer are equivalent and distinct from the system with the spin constraint applied to the entire system (A B Harris 1975, private communication cited in Lubensky and Rubin 1975b). The seeming intractability of a spherical model with an infinite number of constraints has prompted several authors to consider two semi-infinite spherical models. The first has a single overall constraint as in the bulk spherical model (Fisher and Barber 1972, 1973, Barber 1974, Barber *et al* 1974). The second has an overall constraint plus a separate constraint on the surface layer (Singh *et al* 1975). Neither of these models is equivalent to the one considered here and both disagree with the exact results for the n-vector model in d dimensions presented in § 5. This point will be discussed further in § 5.

To summarise, we consider here the $n=\infty$ limit of the continuum model described by the Hamiltonian, equation (1.1) with zero surface field, $h_1=0$. For the moment let us regard the integration over $\boldsymbol{x}$ in equation (1.1) as extending over all space. Our aim is to compute the spin–spin correlation function

$$G(\boldsymbol{\rho}, z, z') = \langle \phi_i(\boldsymbol{\rho}, z)\phi_i(0, z')\rangle = \frac{\int \mathrm{D}\phi\, \phi_i(\boldsymbol{\rho}, z)\phi_i(0, z')\exp(-H)}{\int \mathrm{D}\phi\, \exp(-H)} \tag{3.1}$$

where $(\boldsymbol{\rho}, z)$ is a parametrisation of the position vector $\boldsymbol{x}$ in which z is a coordinate perpendicular to the surface and $\boldsymbol{\rho}$ is a $(d-1)$-dimensional vector giving position in a plane parallel to the surface. Translational invariance parallel to the surface implies that G only depends on the separation of the spins parallel to the surface, but depends separately on z and z', as indicated in equation (3.1). Note that $\int \mathrm{D}\phi \ldots$ means a functional integration over all order parameter configurations, and that G is independent of i due to the spin isotropy of the model.

The first step is to compute the mean-field correlation function (or 'propagator') $g(\boldsymbol{\rho}, z, z')$ corresponding to the case $u=0$ in equation (1.1). It is convenient to utilise the translational invariance parallel to the surface by introducing the $(d-1)$-dimensional Fourier transform $\hat{\phi}_i(\boldsymbol{k}, z)$ of the order parameter, in terms of which the Hamiltonian becomes (with $u=0=h_1$)

$$H_0 = \int_{-\infty}^{\infty} \mathrm{d}z \sum_{\boldsymbol{k}} \sum_{i=1}^{n} \left[\tfrac{1}{2}(t+k^2+c\delta(z))\hat{\phi}_i(\boldsymbol{k}, z)\hat{\phi}_i(-\boldsymbol{k}, z) + \tfrac{1}{2}\left(\frac{\mathrm{d}\hat{\phi}_i}{\mathrm{d}z}\right)^2\right]. \tag{3.2}$$

If we neglect the term in c, i.e. the 'surface' term, the Hamiltonian may be diagonalised by introducing the Fourier transform with respect to z, $\hat{\phi}_i(\boldsymbol{k}, k_\perp)$, to give

$$H_0^{(0)} = \sum_{\boldsymbol{k}} \sum_{k_\perp} \sum_{i=1}^{n} \tfrac{1}{2}(t+k^2+k_\perp^2)\hat{\phi}_i(\boldsymbol{k}, k_\perp)\hat{\phi}_i(-\boldsymbol{k}, -k_\perp) \tag{3.3}$$

which is the standard 'Gaussian model'. The corresponding correlation function is

$$\hat{g}_{\boldsymbol{k}}^{(0)}(k_\perp) = \langle \hat{\phi}_i(\boldsymbol{k}, k_\perp)\hat{\phi}_i(-\boldsymbol{k}, -k_\perp)\rangle = (t+k^2+k_\perp^2)^{-1} \tag{3.4}$$

with Fourier transform

$$\hat{g}_{\boldsymbol{k}}^{(0)}(z, z') = (1/2\kappa)\exp(-\kappa|z-z'|) \tag{3.5}$$

where

$$\kappa = (t+k^2)^{1/2}. \tag{3.6}$$

The 'surface' term in equation (3.2) is now introduced as a perturbation. Graphical methods are most convenient, as shown in figure 1. The single line is the bulk propagator, equation (3.5), the cross carries a factor $(-c)$ and the double line is the result of summing all orders in c. The result is

$$\hat{g}_k(z, z') = \hat{g}_k^{(0)}(z, z') - c\hat{g}_k^{(0)}(z, 0)\hat{g}_k(0, z'). \tag{3.7}$$

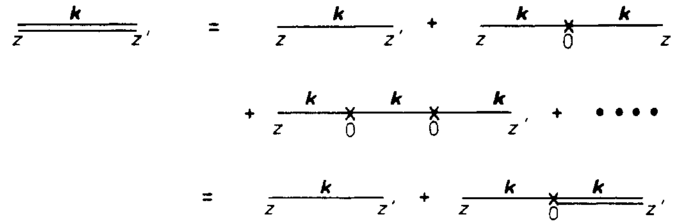

Figure 1. Graphical expansion of the mean-field correlation function in powers of c.

Setting $z = 0$ yields an algebraic equation for $\hat{g}_k(0, z')$:

$$\begin{aligned}\hat{g}_k(0, z') &= \hat{g}_k^{(0)}(0, z') - c\hat{g}_k^{(0)}(0, 0)\hat{g}_k(0, z')\\ &= \hat{g}_k^{(0)}(0, z')(1 + c\hat{g}_k^{(0)}(0, 0))^{-1}.\end{aligned} \tag{3.8}$$

Substituting in equation (3.7) yields

$$\begin{aligned}\hat{g}_k(z, z') &= \hat{g}_k^{(0)}(z, z') - c(1 + c\hat{g}_k^{(0)}(0, 0))^{-1}\hat{g}_k^{(0)}(z, 0)\hat{g}_k^{(0)}(0, z')\\ &= \frac{1}{2\kappa}\left(\exp(-\kappa|z - z'|) - \frac{c}{c + 2\kappa}\exp[-\kappa(|z| + |z'|)]\right),\end{aligned} \tag{3.9a}$$

using equation (3.5). For a semi-infinite system the equivalent result is (LR)

$$\hat{g}_k^{\mathrm{SI}}(z, z') = \frac{1}{2\kappa}\left(\exp(-\kappa|z - z'|) - \frac{c - \kappa}{c + \kappa}\exp[-\kappa(z + z')]\right). \tag{3.9b}$$

To make progress for the case $u \neq 0$, we have found it necessary to remove from the problem as many lengths as possible. To this end we set $t = 0$ (i.e. work at the critical point) and take the limit $c \to \infty$. Thus we set the correlation length equal to infinity and the 'extrapolation length' equal to zero, to obtain

$$\hat{g}_k(z, z') = \frac{1}{2k}\{\exp(-k|z - z'|) - \exp[-k(z + z')]\} = \frac{1}{k}f(kz, kz') \tag{3.10}$$

for both infinite and semi-infinite systems, provided $z, z' \geqslant 0$. Thus the infinite and semi-infinite systems are exactly equivalent for $c = \infty$. (Note that for $c = \infty$ equation (3.9a) implies $\hat{g}_k(z, z') = 0$ if $z > 0$, $z' < 0$ or *vice versa*, so that the two half spaces 'decouple' in this limit.) Observe that for $t = 0$ one recovers equation (3.10) from equations (3.9) for arbitrary c, provided that one is in the scaling regime $k \ll c$. Taking the limit $c \to \infty$ is simply a device for expanding the scaling regime, so that the simple scaling form equation (3.10) holds for all k.

In the large n limit, the quartic term in equation (1.1) is conveniently written as

$$H_1 = \frac{u_0}{4n}\int \mathrm{d}^d x\left(\sum_{i=1}^{n}\phi_i^2(\boldsymbol{x})\right)^2 \tag{3.11}$$

where we have put $u = u_0/n$ to ensure that the correlation function is independent of n in the limit $n \to \infty$. This term is a perturbation to the Hamiltonian H_0 of equation (3.2) and is represented by a four-point interaction in a graphical perturbation expansion. For $n = \infty$, only graphs with the maximal number of closed loops contribute at each order in u_0, since each closed loop carries a factor n (from a sum over spin labels) which exactly cancels the factor $1/n$ associated with each vertex. Hence for $n = \infty$ the full correlation function satisfies the equation represented graphically in figure 2, where a single line is now the mean-field propagator, equation (3.10), the dot carries a factor $(-u_0)$ and the double line is the result of summing to all orders in u_0.

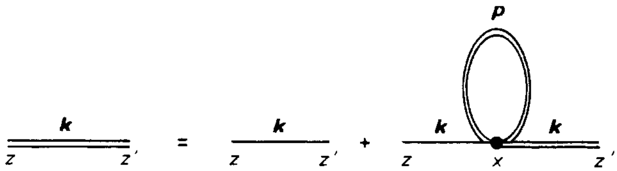

Figure 2. Graphical equation for the exact correlation function for $n = \infty$.

The exact correlation function $\hat{G}_k(z, z')$ thus satisfies the integral equation

$$\hat{G}_k(z, z') = \hat{g}_k(z, z') - \int_0^\infty \mathrm{d}x\, V(x) \hat{g}_k(z, x) \hat{G}_k(x, z') \tag{3.12}$$

where the potential $V(x)$ is the loop in figure 2:

$$V(x) = u_0 \sum_{p<\Lambda} (\hat{G}_p(x, x) - \hat{G}_p(\infty, \infty)). \tag{3.13}$$

Two comments are required here. Firstly, the second term in equation (3.13) is a 'mass subtraction' designed to compensate for the shift in the bulk T_c introduced by the quartic term equation (3.11). It corresponds to replacing t by $t - u_0\langle\phi^2(\infty)\rangle$ in equation (3.2). With this replacement, the bulk critical point remains at $t = 0$ for non-zero u_0. Secondly, Λ in equation (3.13) is a large momentum cut-off for momenta parallel to the surface. Since the cut-off has been taken infinite for the perpendicular momentum component $k_\perp$ (e.g. in going from equation (3.4) to equation (3.5)), the Brillouin zone employed is an infinitely long right-circular cylinder of radius Λ.

The integral equation (3.12) may be converted to a differential equation by taking two derivatives with respect to z and noting that, from equation (3.10),

$$\frac{\mathrm{d}^2 \hat{g}_k(z, z')}{\mathrm{d}z^2} = k^2 \hat{g}_k(z, z') - \delta(z - z'). \tag{3.14}$$

Thus one obtains

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}z^2} - k^2 - V(z)\right) \hat{G}_k(z, z') = -\delta(z - z'). \tag{3.15}$$

By analogy with equation (3.10), we seek a solution of scaling form:

$$\hat{G}_k(z, z') = (1/k) F(kz, kz'). \tag{3.16}$$

Dimensional analysis of equation (3.15) shows that such a solution is only possible if $V(z) \propto z^{-2}$. Therefore we write

$$V(z) = (\mu^2 - \tfrac{1}{4})/z^2, \tag{3.17}$$

where μ is as yet undetermined. Equation (3.15) may now be solved in terms of modified Bessel functions (Abramowitz and Stegun 1965):

$$\hat{G}_{\boldsymbol{k}}(z, z') = (zz')^{1/2} I_\mu(kz) K_\mu(kz'), \qquad z < z' \tag{3.18a}$$

$$\hat{G}_{\boldsymbol{k}}(z, z') = (zz')^{1/2} K_\mu(kz) I_\mu(kz'), \qquad z > z'. \tag{3.18b}$$

In principle a term like $(zz')^{1/2} I_\mu(kz) I_\mu(kz')$ could be added to the right-hand sides of both equations (3.18). It is excluded by the boundary condition that the bulk correlation function $\hat{G}_{\boldsymbol{k}}(\infty, \infty) = 1/2k$ is recovered as $z, z' \to \infty$. It might also be thought that a term like $(zz')^{1/2} K_\mu(kz) K_\mu(kz')$ could be added to both equations since it vanishes at infinity. Addition of such a term is precluded, however, by a rather subtle point which is most easily made by examining the eigenfunctions $\psi(\boldsymbol{k}, \boldsymbol{\rho}, q, z)$ of the linear operator in equation (3.15). These satisfy the equation

$$[\nabla^2 + k^2 + q^2 - (\mu^2 - \tfrac{1}{4})/z^2]\psi = 0. \tag{3.19}$$

The eigenfunctions corresponding to the eigenvalue $(k^2 + q^2)$ are

$$\sqrt{\pi q z} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\rho}) J_\mu(qz) \qquad \text{and} \qquad \sqrt{\pi q z} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\rho}) J_{-\mu}(qz).$$

Note that linear combinations with different q values are not orthogonal, so that mixtures of the eigenfunctions form an over-complete set of states. The only satisfactory orthonormal functions are the given pure eigenfunctions. This situation occurs generally for potentials as or more singular than z^{-2} (Case 1950). The expression for $\hat{G}_{\boldsymbol{k}}(z, z')$ in equations (3.18) then results from the use of the standard relation between the Green function and the eigenfunctions,

$$\hat{G}_{\boldsymbol{k}}(z, z') = \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{q^2 + k^2} \psi(\boldsymbol{k}, \boldsymbol{\rho}, q, z) \psi^*(\boldsymbol{k}, \boldsymbol{\rho}, q, z') \tag{3.20}$$

when the eigenfunction associated with the Bessel function of index μ is substituted for ψ. Only improper linear combinations of eigenfunctions give rise to terms in $\hat{G}$ like $(zz')^{1/2} K_\mu(kz) K_\mu(kz')$, so we can conclude that such terms are absent.

It is convenient to rewrite the expression for the potential $V(z)$ in equation (3.13) as the sum of two terms, $V(z) = V_1(z) + V_2(z)$, where

$$V_1(z) = u_0 \sum_{\text{all } p} (\hat{G}_{\boldsymbol{p}}(z, z) - \hat{G}_{\boldsymbol{p}}(\infty, \infty)) \tag{3.21a}$$

$$V_2(z) = -u_0 \sum_{p > \Lambda} (\hat{G}_{\boldsymbol{p}}(z, z) - \hat{G}_{\boldsymbol{p}}(\infty, \infty)). \tag{3.21b}$$

Inserting the solution, equation (3.18), into equation (3.21) yields

$$V_1(z) = \frac{u_0 K_{d-1}}{z^{d-2}} \int_0^\infty \mathrm{d}t\, t^{d-3} (t I_\mu(t) K_\mu(t) - \tfrac{1}{2}) \tag{3.22}$$

$$V_2(z) = -\frac{u_0 K_{d-1}}{z^{d-2}} \int_{\Lambda z}^\infty \mathrm{d}t\, t^{d-3} (t I_\mu(t) K_\mu(t) - \tfrac{1}{2}) \tag{3.23}$$

where

$$K_{d-1} = 2/\{(4\pi)^{(d-1)/2} \Gamma[(d-1)/2]\}$$

and $\Gamma(x)$ is the gamma function. Using the asymptotic expansion of the product $I_\mu(t)K_\mu(t)$ for large argument yields

$$V_2(z)=\frac{u_0K_{d-1}}{z^{d-2}}\int_{\Lambda z}^{\infty}\mathrm{d}t\,t^{d-3}\left(\frac{4\mu^2-1}{16t^2}+\mathrm{O}(t^{-4})\right)$$

$$=\frac{u_0K_{d-1}}{4\epsilon\Lambda^\epsilon}\frac{\mu^2-\frac{1}{4}}{z^2}+\mathrm{O}\left(\frac{u}{\Lambda^{2+\epsilon}z^4}\right) \tag{3.24}$$

where $\epsilon=4-d$ as usual. Let us neglect for the moment the terms of $\mathrm{O}(u/\Lambda^{2+\epsilon}z^4)$ in equation (3.24). Then for $V(z)$ to have the assumed form, equation (3.17), we require firstly that $V_1(z)$ vanish, since it has the 'wrong' z dependence. The vanishing of the integral in equation (3.22) determines μ. Secondly, we require for consistency that the coupling constant u_0 have a particular value:

$$u_0=u_{\mathrm{W}}=4\epsilon\Lambda^\epsilon/K_{d-1}. \tag{3.25}$$

This special choice of coupling constant removes 'slow transients' of relative order $(k/\Lambda)^\epsilon$ from the correlation function and its choice is analogous to the special choice of coupling constant in Wilson's ϵ-expansion technique for bulk systems (Wilson 1972). In fact, u_{W} is identical to Wilson's 'magic' value for an $n=\infty$ bulk system with the same Brillouin zone as that used here, namely, an infinitely long cylinder of radius Λ. The choice $u_0=u_{\mathrm{W}}$ is similar in motivation to the choice $c=\infty$ which we made earlier: it is a convenience designed to expand the scaling regime and increase the range of validity of the simple scaling form, equation (3.16). Note that the scaling regime can be expanded to infinity, so that equation (3.18) becomes exact for all k, z and z', by choosing the 'surface potential' to exactly cancel the terms of $\mathrm{O}(u/\Lambda^{2+\epsilon}z^4)$ which we neglected in equation (3.24). This means replacing, in the semi-infinite model described by the Hamiltonian of equation (1.1), the 'surface potential' $c\delta(z)$ by $v(z)$ where

$$v(z)=(\mu^2-\tfrac{1}{4})/z^2-V_2(z). \tag{3.26}$$

Then the effective potential obtained by combining the surface potential with that due to the loop insertion in figure 2 is $v(z)+V_2(z)=(\mu^2-\frac{1}{4})/z^2$, yielding equation (3.18) as an exact result for all k, z and z'. Then the propagator $\hat{g}_k(z,z')$ in equation (3.12) is the mean-field propagator for the surface potential $v(z)$. For a general short-range surface potential of range $\sim\Lambda^{-1}$ (i.e. of the order of a lattice spacing) the result, equation (3.18), is restricted to the scaling regime $z\Lambda$, $z'\Lambda\gg1$, $k/\Lambda\ll1$. We have shown elsewhere (Bray and Moore 1977a) that in this context a 'short range' surface potential is one which decays faster than z^{-2} at large z. All such potentials are expected to produce identical critical exponents and, in the scaling regime, identical correlation functions.

It remains to determine the value of the Bessel function index μ. It is fixed by the condition that the integral in equation (3.22) should vanish. This integral is evaluated in the appendix. The result is

$$\int_0^\infty \mathrm{d}t\,t^{d-3}(tI_\mu(t)K_\mu(t)-\tfrac{1}{2})=\frac{\Gamma(3-d)\Gamma[\frac{1}{2}(d-1)+\mu]\Gamma[\frac{1}{2}(d-1)]}{2^{3-d}(2-d)\Gamma[\frac{1}{2}(3-d)]\Gamma[\mu+\frac{1}{2}(3-d)]}. \tag{3.27}$$

The validity of equation (3.27) is restricted, by the requirement that the integral converges at its upper and lower limits, to dimensionalities d satisfying

$$\max(2, 1-2\mu) < d < 4. \tag{3.28}$$

Zeros of the right-hand side of equation (3.27) occur at $\mu + \frac{1}{2}(3-d) = 0, -1, -2, \ldots$. Only the values 0 and -1, however, are compatible with equation (3.28), which yields ranges $2 < d < 4$ and $3 < d < 4$ for $\mu + \frac{1}{2}(3-d) = 0, -1$, respectively. Hence the two possible solutions, and their ranges of applicability, are

$$\mu = (d-3)/2, \qquad 2 < d < 4 \tag{3.29}$$

and

$$\mu = (d-5)/2, \qquad 3 < d < 4. \tag{3.30}$$

3.1. *The ordinary transition*

The solution $\mu = (d-3)/2$, equation (3.29), is identified with the ordinary transition. To see this one observes that for $d = 4$ the special value of the coupling constant chosen here, u_W, vanishes (equation (3.25)). Therefore, for $d = 4$ the present theory should reproduce the mean-field theory result, equation (3.10). This singles out the root $\mu = (d-3)/2$ since equation (3.18) with $\mu = \frac{1}{2}$ gives equation (3.10). (Note, however, that mean-field theory is not exact for $d = 4$: there are logarithmic corrections. Hence the inequalities $d < 4$ in equations (3.29) and (3.30).)

The correlation function in real space is obtained by setting $\mu = (d-3)/2$ in equations (3.18) and taking the Fourier transform. The result is†

$$\begin{aligned} G(\rho, z, z') &= \tfrac{1}{2}\Gamma(d-2)K_{d-1}\left(\frac{4zz'}{[\rho^2 + (z-z')^2][\rho^2 + (z+z')^2]}\right)^{(d-2)/2} \\ &= \tfrac{1}{2}\Gamma(d-2)K_{d-1}\left(\frac{1}{\rho^2 + (z-z')^2} - \frac{1}{\rho^2 + (z+z')^2}\right)^{(d-2)/2} \end{aligned} \tag{3.31}$$

The final result is remarkably simple: $\rho^2 + (z-z')^2$ is the square of the distance between the spins and $\rho^2 + (z+z')^2$ is the square of the 'image' distance—the distance between one spin and the reflection of the other in the plane $z = 0$. The bulk correlation function for $n = \infty$ is simply equation (3.31) with the 'image' term missing. Three limiting cases of equation (3.31) are of special interest.

Case 1. $z, z' \to \infty$ with ρ, $z - z'$ fixed.
In this limit

$$G(\rho, z, z') \propto \frac{1}{[\rho^2 + (z-z')^2]^{(d-2)/2}},$$

the usual bulk result with bulk exponent $\eta = 0$.

Case 2. $z' \to \infty$ with ρ, z fixed.
In this limit

$$G(\rho, z, z') \propto \frac{1}{z'^{3(d-2)/2}} = \frac{1}{z'^{d-2+\eta_\perp}},$$

† The angular integral is straightforward and the radial integral may be found in Gradshteyn and Ryzhik (1965).

defining the critical exponent $\eta_\perp$, given for $n=\infty$ by

$$\eta_\perp = \tfrac{1}{2}(d-2). \tag{3.32}$$

Case 3. $\rho\to\infty$ with z, z' fixed.
In this limit

$$G(\rho, z, z') \propto \frac{1}{\rho^{2(d-2)}} = \frac{1}{\rho^{d-2+\eta_\parallel}}$$

defining the critical exponent $\eta_\parallel$, given for $n=\infty$ by

$$\eta_\parallel = d-2. \tag{3.33}$$

The exponents $\eta_\perp$ and $\eta_\parallel$ for the ordinary transition have been computed to $O(\epsilon)$, for arbitrary n, by Lubensky and Rubin (1975b):

$$\eta_\perp = 1 - \tfrac{1}{2}\left(\frac{n+2}{n+8}\right)\epsilon + O(\epsilon^2) \tag{3.34a}$$

$$\eta_\parallel = 2 - \left(\frac{n+2}{n+8}\right)\epsilon + O(\epsilon^2). \tag{3.34b}$$

For $n=\infty$ equations (3.34) reduce exactly to equations (3.32) and (3.33), indicating that the $O(\epsilon^2)$ terms in equations (3.34) are $O(1/n)$. Lubensky and Rubin also calculated the spin–spin correlation function at $T=T_c$ to $O(\epsilon)$. On the basis of their result they conjectured that $G(\boldsymbol{\rho}, z, z')$ has in general the form

$$G(\boldsymbol{\rho}, z, z') = \text{constant} \times \left[\frac{1}{r^{d-2+\eta}}\left(\frac{\bar{r}^2}{4zz'}\right)^{\bar{\eta}} - \frac{1}{\bar{r}^{d-2+\eta}}\left(\frac{r^2}{4zz'}\right)^{\bar{\eta}}\right] \tag{3.35}$$

where

$$r^2 = (z-z')^2 + \rho^2, \qquad \bar{r}^2 = (z+z')^2 + \rho^2, \qquad \bar{\eta} = \frac{1}{2}\left(\frac{n+2}{n+8}\right)\epsilon + O(\epsilon^2).$$

For $n=\infty$, this result reduces, after some rearrangement of terms, to equation (3.31). Hence the Lubensky–Rubin conjecture is confirmed, for arbitrary dimensionality, for the case $n=\infty$.

3.2. *The special transition*

The solution $\mu=(d-5)/2$, equation (3.30), is identified with the special transition. Recall that in mean-field theory, the special transition corresponds to a semi-infinite system with $c=0$ (an infinite system with $c=0$ gives, of course, the bulk transition). The mean-field propagator at the special transition is, therefore, obtained by putting $c=0$, $\kappa=k$ in equation (3.9b):

$$\hat{g}_k(z, z') = (1/2k)\{\exp(-k|z-z'|) + \exp[-k(z+z')]\}, \tag{3.36}$$

which differs from equation (3.10) in the sign of the second ('image') term. Nevertheless, this $\hat{g}_k(z, z')$ is of scaling form and satisfies equation (3.14) so that the arguments leading to equations (3.18) still hold. For $d=4$, equations (3.18) should reduce to equation (3.36), which implies that $\mu=-\frac{1}{2}$ and singles out the root $\mu=(d-5)/2$ for the special transition.

The restriction to dimensionalities in the range $3<d<4$ in equation (3.30) is easy to understand physically. The special transition corresponds to a surface potential which is not quite attractive enough to split off a surface phase. In a sense it represents a borderline between ordinary and surface transitions. Now for $n=\infty$ and $d\leqslant 3$ the surface transition does not exist (see § 5) since the $(d-1)$-dimensional system does not order. Therefore, the special transition does not exist either and the ordinary transition is observed for all surface potentials.

For $\mu=(d-5)/2$, the Fourier transform of $G_k(z, z')$ cannot be written in a simple form like equation (3.31). The critical exponent $\eta_\|^{\mathrm{sp}}$, however, can be obtained directly from equations (3.18) which give, for $\mu<0$ and $k\to 0$ with z, z' fixed:

$$\begin{aligned}&\hat{G}_k(z, z')\sim(zz')^{1/2}(kz)^{-|\mu|}(kz')^{-|\mu|}, \qquad k\to 0\\&\hat{G}_k(z, z')\propto k^{-2|\mu|},\end{aligned} \tag{3.37}$$

(since $I_\mu(x)\sim x^\mu$, $K_\mu(x)\sim x^{-|\mu|}$ as $x\to 0$). Therefore, for $\rho\to\infty$ at fixed z, z' we deduce that

$$G(\boldsymbol{\rho}, z, z')\propto\frac{1}{\rho^{d-1+2\mu}}, \qquad \rho\to\infty \tag{3.38}$$

giving

$$\eta_\|^{\mathrm{sp}}=1+2\mu \tag{3.39}$$

or

$$\eta_\|^{\mathrm{sp}}=d-4. \tag{3.40}$$

A similar argument for $\mu>0$ shows that equation (3.38) is valid regardless of the sign of μ (e.g. $\mu=(d-3)/2$ gives $\eta_\|=d-2$, the correct result for the ordinary transition). The value of $\eta_\perp$ may be deduced from that of $\eta_\|$ by using the scaling law (Lubensky and Rubin 1975b, and § 5) $\eta_\|=2\eta_\perp-\eta$ to give

$$\eta_\perp^{\mathrm{sp}}=\tfrac{1}{2}(d-4). \tag{3.41}$$

3.3. *The extraordinary transition*

The extraordinary transition occurs at $T=T_c$ as the bulk orders in the presence of an ordered surface. Translational invariance parallel to the surface implies that the magnetisation density (which we assume to be parallel to the '1' direction in spin space) depends only on the distance z from the surface, $\langle\phi_1(\boldsymbol{x})\rangle=m(z)$. Accordingly we write

$$\phi_1(\boldsymbol{x})=m(z)+p(\boldsymbol{x}) \tag{3.42}$$

and determine $m(z)$ from the condition

$$\langle p(\boldsymbol{x})\rangle=0. \tag{3.43}$$

Substituting equation (3.42) into equation (1.1) yields (with $u = u_0/n$)

$$H = \text{constant} + \int \mathrm{d}^d x \Big[\tfrac{1}{2}(t + u_0 m^2(z)) \sum_{i=2}^{n} \phi_i^2(\boldsymbol{x}) + \tfrac{1}{2} \sum_{i=2}^{n} (\nabla\phi_i)^2$$
$$+ \tfrac{1}{2}(t + 3u_0 m^2(z))p^2 + \tfrac{1}{2}(\nabla p)^2$$
$$+ \frac{u_0 m(z)}{\sqrt{n}} p \Big(\sum_{i=2}^{n} \phi_i^2 + p^2 \Big) + \frac{u_0}{4n} \Big(\sum_{i=2}^{n} \phi_i^2 + p^2 \Big)^2$$
$$+ \sqrt{(n)} p (t m(z) + u_0 m^3(z)) + \sqrt{(n)} \nabla p \cdot \nabla m \Big]$$
$$+ \text{surface terms} \tag{3.44}$$

where the constant contains contributions to H which are independent of $p(\boldsymbol{x})$ and $\phi_i(\boldsymbol{x})$, and 'surface terms' are the terms in equation (1.1) which involve $\delta(z)$. The final term in equation (3.44) may be integrated by parts:

$$\int \mathrm{d}^d x \nabla p \cdot \nabla m = \int \mathrm{d}^d x \frac{\mathrm{d}p}{\mathrm{d}z} \frac{\mathrm{d}m}{\mathrm{d}z} = \text{surface term} - \int \mathrm{d}^d x p(\boldsymbol{x}) \frac{\mathrm{d}^2 m}{\mathrm{d}z^2}. \tag{3.45}$$

The broken spin symmetry implied by the ordered surface means that there are two spin–spin correlation functions associated with the extraordinary transition: the 'longitudinal' and 'transverse' functions

$$G^{\mathrm{L}}(\boldsymbol{\rho}, z, z') = \langle p(\boldsymbol{\rho}, z) p(0, z') \rangle$$
$$G^{\mathrm{T}}(\boldsymbol{\rho}, z, z') = \langle \phi_1(\boldsymbol{\rho}, z) \phi_i(0, z') \rangle, \qquad i \geq 2.$$

In this section we will discuss only transverse correlations. The longitudinal correlation function may be calculated in principle, but the computational problems are comparable to those encountered in the computation to order $1/n$ of the correlation function at the ordinary transition.

By analogy with the treatment of the ordinary and special transitions, we seek a solution for $\hat{G}_{\boldsymbol{k}}^{\mathrm{T}}(z, z')$ in the scaling form of equation (3.16). To this end we set $t = 0$ in equation (3.44) and take the limit $c \to -\infty$. The 'bare' propagators for both longitudinal and transverse fluctuations are then given by equation (3.10). These are the propagators derived from equation (3.44) when only the $(\nabla p)^2$, $(\nabla\phi_i)^2$ and surface terms are taken into account. The remaining terms, which are linear, quadratic, cubic and quartic in p and ϕ_i $(i \geq 2)$ are treated by graphical perturbation theory. The various types of vertices, and their associated factors, are given in figure 3. The magnetisation density $m(z)$ is determined by equation (3.43) which is given in terms of graphs, for $n = \infty$, by figure 4. Using the identifications given in figure 3, we derive the equation

$$\frac{\mathrm{d}^2 m}{\mathrm{d}z^2} = m(z) \Big(u_0 m^2(z) + u_0 \sum_{p<\Lambda} (\hat{G}_{\boldsymbol{p}}^{\mathrm{T}}(x, x) - \hat{G}_{\boldsymbol{p}}^{\mathrm{T}}(\infty, \infty)) \Big) \tag{3.46}$$

where, as in equation (3.13), the final term contains a 'mass subtraction' introduced to compensate for the shift in T_{c} when u_0 is non-zero.

The transverse correlation function for $n = \infty$ is given by the graphs of figure 5. Using figure 3, we can write down the integral equation:

$$\hat{G}_{\boldsymbol{k}}^{\mathrm{T}}(z, z') = \hat{g}_{\boldsymbol{k}}(z, z') - \int_0^\infty \mathrm{d}x \, V(x) \hat{g}_{\boldsymbol{k}}(z, x) \hat{G}_{\boldsymbol{k}}^{\mathrm{T}}(x, z') \tag{3.47}$$

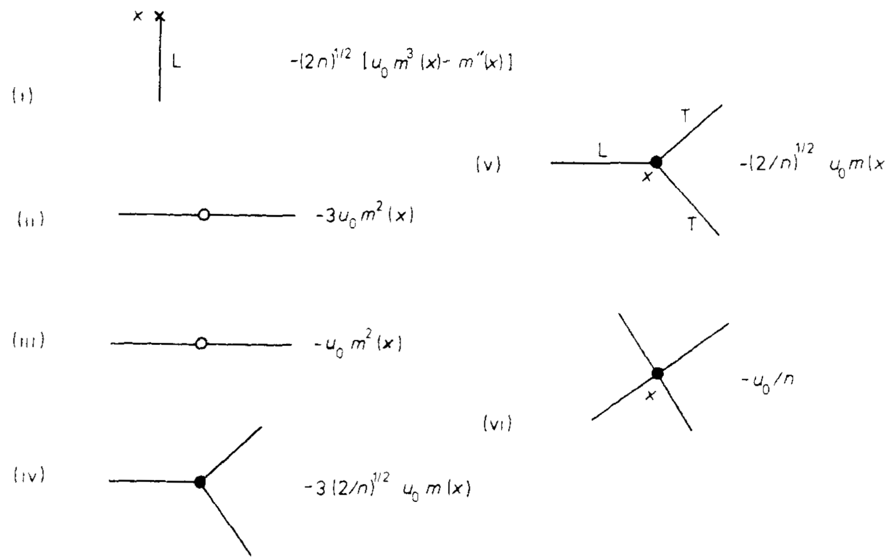

Figure 3. Various vertices appearing in the graphical expansions for the magnetisation density and correlation functions at the extraordinary transition, with their associated factors. L and T refer to longitudinal and transverse propagators respectively.

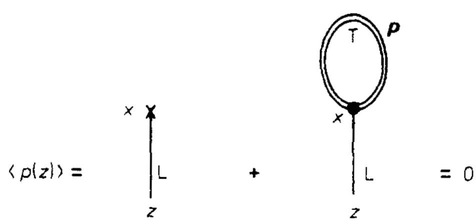

Figure 4. Graphs for $\langle p(z)\rangle$ for $n=\infty$. This equation determines $m(z)$ at the extraordinary transition. The double line is the exact transverse correlation function for $n=\infty$. The single line is the longitudinal propagator, in which insertions of types (ii) and (vi) (figure 3) have been implicitly included (type (iv) insertions do not appear for $n=\infty$).

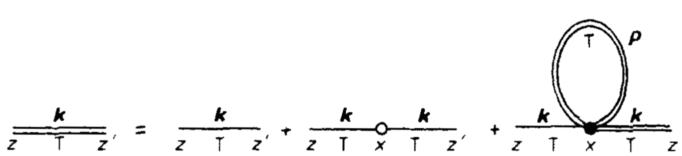

Figure 5. Graphical equation for the transverse correlation function at the extraordinary transition for $n=\infty$.

which has a form identical to that of equation (3.12), except that now the potential $V(x)$ is given by

$$V(x)=u_0m^2(x)+u_0\sum_{p<\Lambda}(\hat{G}_p^{\mathrm{T}}(x,x)-\hat{G}_p^{\mathrm{T}}(\infty,\infty)), \tag{3.48}$$

making the usual mass subtraction. Note that equations (3.46) and (3.48) can be combined to give

$$d^2m/dz^2 = V(z)m. \tag{3.49}$$

In the usual way we require that $V(z) = (\mu^2 - \frac{1}{4})/z^2$. Then the solution is given by equations (3.18) and it only remains to determine μ. To do this we rearrange equation (3.48) as

$$V(x) = u_0\Big(m^2(x) + \sum_{\text{all } p} (\hat{G}_p^{\mathrm{T}}(x, x) - \hat{G}_p^{\mathrm{T}}(\infty, \infty))\Big) - u_0 \sum_{p>\Lambda} (\hat{G}_p^{\mathrm{T}}(x, x) - \hat{G}_p^{\mathrm{T}}(\infty, \infty)). \tag{3.50}$$

The final term is just $V_2(x)$ (equation (3.21*b*)) and therefore, with the choice $u_0 = u_{\mathrm{W}}$ it gives, neglecting term of $O(1/\Lambda^2 x^4)$, exactly the desired potential $(\mu^2 - \frac{1}{4})/x^2$ (see equation (3.24)). Hence μ is determined by the vanishing of the expression in square brackets in equation (3.50). Dimensional analysis (compare equation (3.22)) therefore requires that

$$m(x) = A/x^{(d-2)/2}, \tag{3.51}$$

where A is a constant. Substitution into equation (3.49), with $V(z) = (\mu^2 - \frac{1}{4})/z^2$, yields

$$\mu = (d-1)/2, \qquad 2 < d < 4 \tag{3.52}$$

the range of validity being given by equation (3.28). The constant A is determined by demanding that the expression in square brackets vanish in equation (3.50), where the sum over $\boldsymbol{p}$ may be evaluated using equation (3.27). The result is that $A^2 > 0$, as required for a real magnetisation density, for all d in the range $2 < d < 4$.

The exponent $\eta_\parallel$ is given by the general result (cf equation (3.39)) $\eta_\parallel = 1 + 2\mu$, i.e.

$$\eta_\parallel^{\mathrm{e,T}} = d \tag{3.53}$$

where the superscript T indicates that the exponent applies to transverse correlations. It may also be shown that

$$\eta_\perp^{\mathrm{e,T}} = d/2. \tag{3.54}$$

We argue in § 5 that equations (3.53) and (3.54) are exact results.

As usual, mean-field theory is a special case of the present calculation, obtained by setting $d = 4$, i.e. $\mu = 3/2$. The longitudinal correlation function, which is intractable for $n = \infty$, has been computed in mean-field theory by LR who obtain (for zero extrapolation length) equations (3.18) with $\mu = 5/2$, and therefore find the critical exponent $\eta_\parallel^{\mathrm{e,L}} = 1 + 2\mu = 6$. We show in § 5 that the exact result (for all n) is

$$\eta_\parallel^{\mathrm{e,L}} = d + 2. \tag{3.55}$$

All the results presented here have been restricted to the case $T = T_{\mathrm{c}}$. Unfortunately, we can see no way of obtaining exact results away from the bulk critical temperature, and for this reason have been unable to investigate the surface transition in the large n limit. The difficulty lies in the fact that for $T \neq T_{\mathrm{c}}$ an extra length, the correlation length ξ, enters the problem so that the scaling *ansatz*, equation (3.16), becomes invalid. In addition, the potential $V(z)$ presumably becomes temperature dependent. Similar difficulties accompany the generalisation to arbitrary c. At present we can see no way of surmounting these difficulties.

4. The ϵ expansion

Critical exponents for the ordinary transition have been computed to $O(\epsilon)$ by Lubensky and Rubin (1973, 1975b) using the full renormalisation group approach. The ϵ expansion for the extraordinary transition is dogged by severe computational problems owing to the complicated nature of the mean-field propagators, i.e. products of modified Bessel functions. We concentrate here on the special transition, as this is the one case for which we have been unable to find scaling arguments which give the exponents exactly in terms of bulk exponents. The philosophy we adopt is that of the Wilson (1972) perturbation theory technique, in which a special value $u(\epsilon)$ of the coupling constant is used, the value of which is chosen so that the logarithms which appear at each order in ϵ can be identified as the expansion of a simple power law. In addition, we must choose a special value $c=c^*(\epsilon)$ appropriate to the special transition. It is instructive to consider the semi-infinite and infinite problems separately.

4.1. *Semi-infinite problem*

The mean-field propagator for this case is given by equation (3.9*b*). We work at the critical point (i.e. set $\kappa=k$) and for simplicity consider the surface plane $z=0=z'$:

$$\hat{g}_k^{\mathrm{SI}}(0,0)=(c+k)^{-1}. \tag{4.1}$$

The exponent $\eta_\parallel$ may be obtained from the behaviour at small k (compare the arguments leading to equation (3.39)) via the observation that the singular part of the correlation function behaves as $k^{\eta_\parallel-1}$ as $k\to 0$. For any finite c, the small k behaviour in mean-field theory is

$$\hat{g}_k^{\mathrm{SI}}(0,0)=\frac{1}{c}-\frac{k}{c^2}+\dots$$

giving an exponent $\eta_\parallel=2$, the usual mean-field result for the ordinary transition (compare equation (3.33) with $d=4$). The case $c=0$ is special, however, since then $\hat{g}_k^{\mathrm{SI}}(0,0)=1/k$ exactly. This is the special transition (the '$\lambda=\infty$' transition of LR) with mean-field exponent $\eta_\parallel^{\mathrm{sp}}=0$ (compare equation (3.40) with $d=4$).

Outside mean-field theory we expect the value of c appropriate to the special transition, c^*, to be different from zero. Suppose c^* is $O(\epsilon)$. Then equation (4.1) may be expanded, (with $c=c^*$, to $O(\epsilon)$:

$$\hat{g}_k^{\mathrm{SI}}(0,0)=\frac{1}{k}-\frac{c^*}{k^2}+O(\epsilon^2). \tag{4.2}$$

A further $O(\epsilon)$ contribution to the full propagator $\hat{G}_k^{\mathrm{SI}}(0,0)$ is given by the graph of figure 6. The lines are given by equation (3.9*b*) (with $\kappa=k$), and we may take $c=0$ in this graph, rather than $c=c^*$, since the resulting error is $O(\epsilon^2)$. The dot carries a factor $(-u)$, where the Wilson (1972) value of u is $u=8\pi^2\epsilon/(n+8)+O(\epsilon^2)$, even for the cylindrical Brillouin zone used here. The combinatoric factor associated with the

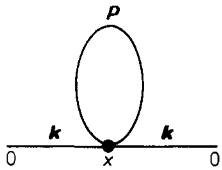

Figure 6. Order ϵ contribution to $\hat{G}_k(0, 0)$.

loop is $(n+2)$. We will make the standard subtraction of the loop at $x=\infty$ to compensate for the T_c shift introduced by the quartic interaction. Hence we obtain

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\hat{g}_k^{\mathrm{SI}}(0,0)-(n+2)u\int_0^\infty \mathrm{d}x\, \hat{g}_k^{\mathrm{SI}}(0,x)\hat{g}_k^{\mathrm{SI}}(x,0)\sum_{p<\Lambda}(\hat{g}_p^{\mathrm{SI}}(x,x)-\hat{g}_p^{\mathrm{SI}}(\infty,\infty))+\mathrm{O}(\epsilon^2) \tag{4.3}$$

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\frac{1}{k}-\frac{c^*}{k^2}-\frac{8\pi^2\epsilon}{k^2}\left(\frac{n+2}{n+8}\right)\int_0^\infty \mathrm{d}x\, \exp(-2kx)\sum_{p<\Lambda}\frac{1}{2p}\exp(-2px)+\mathrm{O}(\epsilon^2) \tag{4.4}$$

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\frac{1}{k}-\frac{c^*}{k^2}-\frac{2\pi^2\epsilon}{k^2}\left(\frac{n+2}{n+8}\right)\sum_{p<\Lambda}\frac{1}{p(p+k)}+\mathrm{O}(\epsilon^2). \tag{4.5}$$

To leading order the sum over $\boldsymbol{p}$ may be evaluated in three dimensions (i.e. the three-dimensional surface of a four-dimensional system) to give

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\frac{1}{k}-\frac{c^*}{k^2}-\frac{\epsilon}{k^2}\left(\frac{n+2}{n+8}\right)\left(\Lambda-k\ln\frac{\Lambda}{k}\right)+\mathrm{O}(\epsilon^2) \tag{4.6}$$

for $\Lambda \gg k$. The strongly divergent term which is linear in the cut-off Λ is eliminated by choosing

$$c^*=-\epsilon\left(\frac{n+2}{n+8}\right)\Lambda+\mathrm{O}(\epsilon^2). \tag{4.7}$$

The remaining two terms in equation (4.6) may be combined to yield

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\frac{1}{k}\left(\frac{\Lambda}{k}\right)^{[(n+2)/(n+8)]\epsilon}+\mathrm{O}(\epsilon^2) \tag{4.8}$$

whence one identifies the critical exponent

$$\eta_\parallel^{\mathrm{sp}}=-[(n+2)/(n+8)]\epsilon+\mathrm{O}(\epsilon^2). \tag{4.9}$$

Note that, for $n=\infty$, this agrees with equation (3.40).

It is interesting, and straightforward, to generalise equation (4.6) to arbitrary c. One simply uses equation (3.9b) (with $\kappa=k$) in equation (4.3), keeping c arbitrary. The result is

$$\hat{G}_k^{\mathrm{SI}}(0,0)=\frac{1}{c+k}-\frac{\epsilon}{(c+k)^2}\left(\frac{n+2}{n+8}\right)\left[\Lambda-\frac{2c^2}{c-k}\ln\left(\frac{\Lambda}{c}+1\right)+\frac{k(c+k)}{c-k}\ln\left(\frac{\Lambda}{k}+1\right)\right]+\mathrm{O}(\epsilon^2). \tag{4.10}$$

Setting $c=c^*$, equation (4.7), and expanding to $\mathrm{O}(\epsilon)$, gives back equation (4.8).

Another case of interest is $k=0$, $c \ll \Lambda$, which gives

$$\hat{G}^{\mathrm{SI}}_{k=0}(0,0) = \frac{1}{c} - \frac{\epsilon}{c^2}\left(\frac{n+2}{n+8}\right)\left(\Lambda - 2c \ln\frac{\Lambda}{c}\right) + \mathrm{O}(\epsilon^2)$$

$$= \frac{1}{c-c^*}\left(\frac{\Lambda}{c-c^*}\right)^{2[(n+2)/(n+8)]\epsilon} + \mathrm{O}(\epsilon^2). \tag{4.11}$$

The exponent which governs the divergence of $\hat{G}_{k=0}(0,0)$ as $c \to c^*$ may be determined by scaling arguments. In addition to the standard scaling correspondence $k \sim t^{\nu}$ we argue in § 5 that there is a scaling correspondence $c - c^* \sim t^{1-\nu}$. Hence the dependence on $c - c^*$ at $t = 0 = k$ follows from

$$\hat{G}^{\mathrm{SI}}_{k=0}(0,0) \sim \frac{1}{k^{1-\eta_{\parallel}^{\mathrm{sp}}}} \sim \frac{1}{t^{\nu(1-\eta_{\parallel}^{\mathrm{sp}})}} \sim \frac{1}{(c-c^*)^{\nu(1-\eta_{\parallel}^{\mathrm{sp}})/(1-\nu)}}. \tag{4.12}$$

According to equation (4.11) we have

$$\frac{\nu}{1-\nu}(1-\eta_{\parallel}^{\mathrm{sp}}) = 1 + 2\epsilon\left(\frac{n+2}{n+8}\right) + \mathrm{O}(\epsilon^2)$$

which, using the standard result (Wilson 1972)

$$\nu = \frac{1}{2} + \frac{1}{4}\left(\frac{n+2}{n+8}\right)\epsilon + \mathrm{O}(\epsilon^2),$$

gives back equation (4.9). Thus the scaling correspondence $c - c^* \sim t^{1-\nu}$ is verified to $\mathrm{O}(\epsilon^2)$.

4.2. *Infinite problem*

The computation proceeds exactly as in the semi-infinite case, except that the mean-field propagators are given by equation (3.9*a*) instead of equation (3.9*b*), and the integration over x in equation (4.3) extends from $-\infty$ to ∞ instead of from 0 to ∞. The analogue of equation (4.10) for the infinite problem is

$$\hat{G}_k(0,0) = \frac{1}{c+2k} + \epsilon\left(\frac{n+2}{n+8}\right)\frac{2c}{(c+2k)^2(c-2k)}\left[\frac{c}{2}\ln\left(\frac{2\Lambda}{c}+1\right) - k\ln\left(\frac{\Lambda}{k}+1\right)\right] + \mathrm{O}(\epsilon^2). \tag{4.13}$$

In contrast to equation (4.10), there is no term linear in the cut-off Λ in equation (4.13). This is because the critical value of c for splitting off a surface phase remains $c=0$ exactly, corresponding to the bulk transition. Setting $c=0$ in equation (4.13) yields $\hat{G}_k(0,0) = 1/k$, the expected bulk result with bulk exponent $\eta = 0$ to $\mathrm{O}(\epsilon)$ (in general $\hat{G}_k(0,0) \sim 1/k^{1-\eta}$). On the other hand, the case $k=0$, $c \ll \Lambda$ yields

$$\hat{G}_{k=0}(0,0) = \frac{1}{c} + \frac{\epsilon}{c}\left(\frac{n+2}{n+8}\right)\ln\left(\frac{2\Lambda}{c}\right) + \mathrm{O}(\epsilon^2)$$

$$= \frac{1}{c}\left(\frac{2\Lambda}{c}\right)^{\epsilon[(n+2)/(n+8)]} + \mathrm{O}(\epsilon^2). \tag{4.14}$$

The scaling correspondences $k \sim t^{\nu}$, $c \sim t^{1-\nu}$ (see § 5) imply that

$$\frac{\nu}{1-\nu}(1-\eta)=1+\epsilon\left(\frac{n+2}{n+8}\right)+O(\epsilon^2),$$

which is readily verified using the standard expansion for ν, and recalling that $\eta=0$ to $O(\epsilon)$.

5. Scaling arguments

5.1. *The ordinary transition*

Scaling relations between the various surface critical exponents have been derived by Fisher (1971, 1973), Binder and Hohenberg (1972, 1974) and Barber (1973a). The basic assumption is that the free energy associated with the surface has the scaling form

$$F_s=|t|^{2-\alpha_s}f\left(\frac{h}{|t|^{\Delta}},\frac{h_1}{|t|^{\Delta_1}}\right) \tag{5.1}$$

where h is a uniform field and h_1 a field applied in the surface only. One distinguishes between 'global' and 'local' quantities. 'Global' quantities, such as the surface free energy F_s, the total surface magnetisation $m_s=\partial F_s/\partial h$ and the total surface susceptibility $\chi_s=\partial^2F_s/\partial h^2$, are proportional to the surface area and diverge with exponents labelled with subscripts 's': $F_s\sim t^{2-\alpha_s}$, $m_s\sim|t|^{\beta_s}$, $\chi_s\sim t^{-\gamma_s}$. 'Local' quantities, e.g. $\chi_{1,1}=\partial^2F/\partial h_1^2$, $\chi_1=\partial^2F/\partial h\partial h_1$, $m_1=\partial F/\partial h_1$, are defined at a point in the surface, and diverge with exponents labelled with subscripts '1': $\chi_{1,1}\sim t^{-\gamma_{1,1}}$, $\chi_1\sim t^{-\gamma_1}$, $m_1\sim|t|^{\beta_1}$.

The 'global' exponents are readily determined in terms of the bulk exponents by the following argument. First, we make the assumption (Binder and Hohenberg 1972, 1974, Barber 1973a, Fisher 1971, 1973) that there is a single diverging correlation length ξ as the critical point is approached. Then the local free energy density $f_s(z)$ is assumed to have the scaling form

$$f_s(z)=t^{2-\alpha}g(z/\xi) \tag{5.2}$$

where $g(\infty)=1$, i.e. the usual bulk result is recovered far from the surface. Then the total free energy associated with the surface is

$$F_s=\int_0^\infty dz\,(f_s(z)-f_s(\infty))=t^{2-\alpha}\int_0^\infty dz\,(g(z/\xi)-1)\propto t^{2-\alpha}\xi\propto t^{2-\alpha-\nu}. \tag{5.3}$$

Therefore one identifies

$$\alpha_s=\alpha+\nu. \tag{5.4}$$

Similar arguments yield

$$\beta_s=\beta-\nu \tag{5.5}$$

$$\gamma_s=\gamma+\nu. \tag{5.6}$$

Relationships between the local exponents are obtained by taking derivatives of F_s, equation (5.1), with respect to the fields h, h_1. Results are (Binder and Hohenberg

1972, 1974, Barber 1973a, Fisher 1971, 1973)

$$\beta_1 + \Delta_1 = 2 - \alpha_s = 2 - \alpha - \nu \tag{5.7}$$

$$\beta_1 + \gamma_{1,1} = \Delta_1 \tag{5.8}$$

$$2\gamma_1 - \gamma_{1,1} = \gamma_s = \gamma + \nu. \tag{5.9}$$

Note that equation (5.8) was derived in § 2 as equation (2.17*a*). The exponent $\delta_{1,1}$ will not be considered explicitly here, but may be derived from $\delta_{1,1} = \Delta_1/\beta_1$, equation (2.17*b*). Scaling relations involving the correlation exponents may be derived by writing the correlation function in scaling form (Binder and Hohenberg 1972) to give

$$\gamma_1 = \nu(2 - \eta_\perp) \tag{5.10}$$

$$\gamma_{1,1} = \nu(1 - \eta_\parallel). \tag{5.11}$$

Combining these with equation (5.9) and using the bulk scaling law $\gamma = \nu(2-\eta)$ yields a relation for the η (Lubensky and Rubin 1975b):

$$\eta_\parallel = 2\eta_\perp - \eta. \tag{5.12}$$

A convenient equation for β_1 may be obtained by adding equations (5.7) and (5.8), substituting for $\gamma_{1,1}$ from equation (5.11), and using the bulk scaling law $2 - \alpha = d\nu$ to give

$$\beta_1 = (\nu/2)(d - 2 + \eta_\parallel), \tag{5.13}$$

a form reminiscent of the bulk scaling law $\beta = (\nu/2)(d - 2 + \eta)$.

It is important to notice that equations (5.7)–(5.11) determine all the surface exponents in terms of bulk exponents if any one surface exponent is known, since they are five independent equations for the six exponents β_1, Δ_1, $\gamma_{1,1}$, γ_1, $\eta_\perp$ and $\eta_\parallel$. In this section we will derive an extra scaling law, $\gamma_{1,1} = \nu - 1$, and thence determine all the surface exponents for the ordinary transition.

The principal theoretical idea is that the characteristic feature of a 'surface' problem is the loss of translational invariance due to the existence of the surface, rather than the semi-infiniteness of the problem. We suggest that all the richness of the theory of phase transitions in semi-infinite systems (with the possible exception of the special transition) may be observed in the bulk system by applying a perturbation which destroys the translational invariance. If this 'surface' perturbation takes the form, as in equation (1.1), of a term which is already present in the bulk Hamiltonian, then it is not surprising that the critical exponents in the presence of the perturbation are expressible in terms of the usual bulk exponents.

We begin by considering the Hamiltonian of equation (1.1) with the integration extending over all space and with $h_1 = 0$ and $c < 0$. If n and d are such that the surface can order at a higher temperature than the bulk, then the surface transition temperature $T_c(c)$ is related to c by the crossover exponent ϕ_s (compare equation (2.24)) according to

$$T_c(c) - T_c(0) \propto |c|^{1/\phi_s} \tag{5.14}$$

as $c \to 0-$. Our results are based on the observation (Bray and Moore 1977b) that ϕ_s may be deduced from the scaling properties of the surface perturbation

$$H_s = \tfrac{1}{2}c \int d^d x\, \delta(z) \sum_{i=1}^{n} \phi_i^2(\boldsymbol{x}) \tag{5.15}$$

under a renormalisation group transformation R (Ma 1973a, b, Fisher 1974, Wilson and Kogut 1974) in which all lengths are scaled by a factor b, i.e. R is the transformation $\boldsymbol{x} \to b\boldsymbol{x}'$. Since $\Sigma_{i=1}^{n} \phi_i^2(\boldsymbol{x})$ is simply the energy density, its singular part $e(\boldsymbol{x})$ behaves in the bulk as $t^{1-\alpha}$, or $\xi^{-(1-\alpha)/\nu}$, and therefore scales as $b^{-(1-\alpha)/\nu}$. Thus

$$e(\boldsymbol{x}) \to b^{-(1-\alpha)/\nu} e'(\boldsymbol{x}' = \boldsymbol{x}/b)$$

and

$$RH_s = \tfrac{1}{2} c b^{d-1-(1-\alpha)/\nu} \int \mathrm{d}^d x' \, \delta(z') e'(\boldsymbol{x}'). \tag{5.16}$$

Hence, under the transformation R, the parameter c is rescaled as

$$c' = b^{d-1-(1-\alpha)/\nu} c = b^{(1-\nu)/\nu} c \tag{5.17}$$

where we have used the bulk scaling law $2-\alpha = d\nu$. According to the standard theory of the renormalisation group (e.g. Fisher 1974), if the parameter g which measures the strength of a perturbation to the Hamiltonian rescales as $g' = b^{\lambda} g$, then the crossover exponent associated with g is $\phi = \nu\lambda$. For the present case, therefore, the crossover exponent is

$$\phi_s = 1 - \nu. \tag{5.18}$$

The same result may be obtained by means of a heuristic argument. Consider a fluctuation which tends to order the system near the plane $z = 0$. The spatial extent of the fluctuation is governed by the correlation length ξ, i.e. the region $-\xi \lesssim z \lesssim \xi$ is ordered. Such a fluctuation increases the bulk free energy (per unit area of the plane $z = 0$) by an approximate amount $t^{2-\alpha}\xi$. For $c < 0$, however, the perturbation H_s acts to reduce the free energy per unit area by an approximate amount $|c| t^{1-\alpha}$, to lowest order in c. Hence the total change of free energy (per unit area) due to the fluctuation is

$$\delta F_s \sim t^{2-\alpha}\xi - |c| t^{1-\alpha} \sim t^{1-\alpha}(t^{1-\nu} - |c|). \tag{5.19}$$

If $t^{1-\nu} < |c|$, so that $\delta F_s < 0$, the fluctuation is energetically favoured and the plane $z = 0$ will order. The critical temperature t_c for the formation of a surface phase therefore satisfies $t_c^{1-\nu} = |c|$ which implies $\phi_s = 1 - \nu$. For $\nu > 1$, $\delta F_s > 0$ for small t so that a fluctuation which orders the surface is energetically unfavourable. We conclude that for $\nu > 1$ no surface phase can exist. The case $\nu = 1$ is marginal. Au-Yang (1973) has shown that the semi-infinite two-dimensional Ising model (which has $\nu = 1$) does not exhibit a surface phase.

Why does equation (5.19) not prove that a surface phase exists whenever $\nu < 1$? The full renormalisation group argument given above indicates that equation (5.19) represents the start of an expansion in power of $c/t^{1-\nu}$. For $\nu < 1$ and t small the higher order terms are important, so that equation (5.19) should be replaced by

$$\delta F_s \sim t^{2-\alpha-\nu} f(c/t^{1-\nu}).$$

If a surface phase exists then δF_s must be negative for small t, and the function $f(x)$ must have a zero at $x = x_0 < 0$. Then the surface critical temperature satisfies $t_c^{1-\nu} = c/x_0$, giving $\phi_s = 1 - \nu$ as before. The terms neglected in equation (5.19) therefore change the magnitude of t_c without affecting its dependence on c. It may happen, however, that $f(x)$ is positive for large x (i.e. small t). Then a fluctuation to a state of surface order is energetically unfavourable and no surface ordering will occur. Note that for $\nu > 1$ the terms neglected in equation (5.19) are negligible for small t so that the statement that there can be no surface ordering for this case is rigorously correct. Indeed, for $\nu > 1$ equation (5.17) shows that the surface Hamiltonian H_s is an 'irrelevant operator' in the renormalisation group sense (e.g. Fisher 1974) since c is reduced by each application of R. Therefore, for $\nu > 1$ and c finite, the infinite system has bulk critical behaviour.

For polymers, which are described by the Hamiltonian of equation (1.1) with $n = 0$, the result equation (5.18) has already been derived by de Gennes (1976) using an intuitive argument (de Gennes predicted $\phi_s = 2/5$, implicitly using $\nu = 3/5$ for polymers). The behaviour of polymers at surfaces may provide an application for surface critical phenomena theory.

We turn now to the computation of the critical exponents for the ordinary transition. We start by considering the local susceptibility $\chi_{1,1}$ which is the $k = 0$, $z = 0$, $z' = 0$ form of the correlation function $\hat{G}_k(z, z')$. In mean-field theory, the latter is given by equation (3.9a), with $\kappa = (t + k^2)^{1/2}$. Thus (see also equation (2.9))

$$\begin{aligned}\chi_{1,1}^{\mathrm{MF}} &= \hat{g}_{k=0}(0, 0) = (c + 2t^{1/2})^{-1} \\ &= \frac{1}{c} - \frac{2t^{1/2}}{c^2} + \mathrm{O}\left(\frac{t}{c^3}\right),\end{aligned} \tag{5.20}$$

which gives the usual result (equation (2.10)) $\gamma_{1,1}^{\mathrm{MF}} = -\frac{1}{2}$. Note that equation (5.20) takes the form of an expression in powers of $1/c$. This is an important and general result, valid beyond mean-field theory. To see this, note that the mean-field propagator, equation (3.9a), has itself an expansion in powers of $1/c$:

$$\begin{aligned}\hat{g}_k(z, z') = {} & (1/2\kappa)\{\exp(-\kappa|z - z'|) - \exp[-\kappa(|z| + |z'|)]\} \\ & + (1/c)\{\exp[-\kappa(|z| + |z'|)]\} + \mathrm{O}(c^{-2}).\end{aligned} \tag{5.21}$$

Furthermore, the mean-field propagator for the semi-infinite problem, equation (3.9b), has a similar expansion in powers of $1/c$, but with coefficients which differ from those in equation (5.21) at order $1/c^2$. To go beyond mean-field theory, we treat the quartic terms in the Hamiltonian of equation (1.1) as a perturbation, and in each order of perturbation theory we replace each mean-field propagator which appears by the expansion equation (5.21). Then, summing to all orders in the perturbation, we obtain a $1/c$ expansion for the exact correlation function $\hat{G}_k(z, z')$, and hence a $1/c$ expansion for $\chi_{1,1}$ of the form

$$\chi_{1,1} = \frac{1}{c} - A\frac{t^{-\gamma_{1,1}}}{c^2} + \text{less singular terms} \tag{5.22}$$

where A is a constant. The exact results from the ϵ expansion, equations (4.10) and (4.13), verify this form for both semi-infinite and infinite problems, if one replaces k by its scaling equivalent t^ν, and both results lead to the same identification $\gamma_{1,1} = -\frac{1}{2} + \frac{1}{4}[(n+2)/(n+8)]\epsilon + \mathrm{O}(\epsilon^2)$. However, $\gamma_{1,1}$ can be determined exactly, since the renormalisation group argument given above implies that the first two terms in equation (5.22) become comparable when $t^{1-\nu} \sim c$. Hence one deduces that

$$\gamma_{1,1} = \nu - 1, \tag{5.23}$$

in agreement with the $\mathrm{O}(\epsilon)$ result above.

All other exponents follow from the scaling laws, (5.7)–(5.13), and the bulk scaling law $2-\alpha=d\nu$. The results are:

$$\gamma_1=\nu+(\gamma-1)/2 \tag{5.24}$$

$$\eta_\perp=1-(\gamma-1)/2\nu \tag{5.25}$$

$$\eta_\parallel=1/\nu \tag{5.26}$$

$$\beta_1=\tfrac{1}{2}+\nu(d-2)/2 \tag{5.27}$$

$$\Delta_1=(1-\alpha)/2. \tag{5.28}$$

Since the surface scaling laws are satisfied in all known cases, any one of the above results will suffice for the purpose of checking with exact results. The most convenient is the result for $\eta_\parallel$, which is known to $O(\epsilon)$ (Lubensky and Rubin 1975b, and equation (3.34*b*)), for $n=\infty$ (equation (3.33)) and for the two-dimensional Ising model (McCoy and Wu 1967) which has $\eta_\parallel=1$. All three exact results agree with equation (5.26).

We have deliberately excluded from these comparisons the spherical model (Fisher and Barber 1972, 1973, Barber 1974, Barber *et al* 1974), which has $\eta_\parallel=2$ for all d. In terms of the continuum model used for the $n=\infty$ limit in § 3, the spherical model with a single overall constraint corresponds to replacing the local potential $V(z)$ by its bulk value $V(\infty)$. This model is unphysical. For $T=T_c$, for example, the surface potential required to effect the replacement of $V(z)$ by $V(\infty)$ is long range, falling off as $1/z^2$ for large z. The critical exponents for such a model differ from those appropriate to a short-range surface potential (Bray and Moore 1977a). The exact results, equations (5.23)–(5.28), are restricted to short-range surface potentials, which fall off faster than $1/z^2$ as $z\to\infty$ (Bray and Moore 1977a).

The exact results derived in this section are based on the recursion relation (5.17) for an infinite system with a perturbation H_s in the plane $z=0$. We now assert that the exponents for the ordinary transition in a semi-infinite system are identical to those of the infinite system. The argument is as follows. The recursion relation (5.17) drives c (for $\nu<1$) to the fixed point value $c=\infty$. ($O(c^2)$ terms neglected on the right-hand side of equation (5.17) could, in principle, lead to a finite fixed point value, but we think this unlikely as it would be hard to understand the physical significance of a finite value.) Therefore, we may as well set $c=\infty$ at the outset. But then the mean-field propagators for the infinite and semi-infinite systems, equations (3.9*a*, *b*), become identical so that the critical behaviour of the two systems is identical, order by order in a perturbation expansion in u, and hence the critical exponents are the same. The crossover exponent ϕ_s is related to $\gamma_{1,1}$ by $\gamma_{1,1}=-\phi_s$, according to the argument leading to equation (5.23), and therefore $\phi_s=1-\nu$ for the semi-infinite system also. For the semi-infinite system, however, equation (5.14) must be modified to read $T_c(c)-T_c(0)\propto(c^*-c)^{1/\phi_s}$, as $c\to c^*-$, where c^* is the value of c appropriate to the special transition. The recursion relation (5.17) reads, for the semi-infinite system

$$(c-c^*)'=b^{d-1-(1-\alpha^{sp})/\nu}(c-c^*) \tag{5.29}$$

where $(1-\alpha^{sp})$ is the exponent describing the singularity in the energy density in the plane $z=0$ at the special transition. The assertion that ϕ_s is the same for infinite and semi-infinite systems implies that $\alpha^{sp}=\alpha$. Note that the validity of the scaling correspondence $c\sim t^{1-\nu}$ was verified to $O(\epsilon)$ for both infinite and semi-infinite systems in § 4.

Finally we note that the explicit form of the quartic term in equation (1.1) was not used in deriving the exact results for the exponents. Equations (5.23)–(5.28) are therefore valid quite generally, provided the appropriate bulk exponents are used.

5.2. *The surface transition*

The critical exponents for the surface transition are simply the bulk exponents for the $(d-1)$-dimensional system. To prove this assertion we observe that, for an infinite system with $c<0$, the recursion relation (5.17) drives c (for $\nu<1$) to the fixed point value $c=-\infty$. Similarly, for a semi-infinite system with $c<c^*$, c is driven (for $\nu<1$) to the fixed point value $c=-\infty$ by the recursion relation (5.29). (Again, terms of $O(c^2)$, $O((c-c^*)^2)$ on the right-hand sides of equations (5.17), (5.29) respectively could drive c to a finite negative value, but, as before, this seems unlikely on physical ground.) Therefore we may as well take the limit $c\to-\infty$ at the outset.

For the infinite system with $c<0$ we write the mean-field propagator, equation (3.9*a*), as

$$\hat{g}_k(z,z')=\frac{1}{2\kappa}\{\exp(-\kappa|z-z'|)-\exp[-\kappa(|z|+|z'|)]\}+\frac{1}{2\kappa-|c|}\exp[-\kappa(|z|+|z'|)],\qquad(5.30)$$

where $\kappa=(t+k^2)^{1/2}$. For $k=0$, the second term has a singularity at the surface critical temperature $t_c=\frac{1}{4}|c|^2$. Therefore we set $t=\frac{1}{4}|c|^2+\tau$ in the second term, which becomes

$$\frac{|c|}{2(\tau+k^2)}\{\exp[-\tfrac{1}{2}|c|(|z|+|z'|)]\}(1+O(c^{-1}))\to 2\delta(|z|+|z'|)(\tau+k^2)^{-1}\qquad(5.31)$$

as $|c|\to\infty$. Hence for $c=-\infty$, $\hat{g}_k(z,z')$ breaks up into two terms, the first of which vanishes when either z or z' is zero, and the second of which vanishes except when both z and z' are zero. Moreover, the second term has the form of a mean-field propagator for a $(d-1)$-dimensional system. Consider a computation of the exact propagator between two spins in the surface, $\hat{G}_k(0,0)$. Then only the contribution, equation (5.31), to the mean-field propagator will contribute to $\hat{G}_k(0,0)$ at each order of u in perturbation theory, since any term involving a propagator between a point in the surface and a point in the bulk will vanish identically. Therefore, provided that the $(d-1)$-dimensional system can order spontaneously at finite temperature, the critical exponents of the surface transition are identical to those of the $(d-1)$-dimensional system. An exactly similar argument goes through for a semi-infinite system.

5.3. *The extraordinary transition*

The extraordinary transition may be viewed simply as a special case of the ordinary transition for which the surface field h_1 is finite. Its critical exponents may be computed exactly by a generalisation of the scaling argument which led to equations (5.4)–(5.6). For a finite surface field h_1, the local free-energy density $f_s(z)$ is assumed to have the scaling form

$$f_s(z)=t^{2-\alpha}g(z/\xi,z/\xi_{h_1})\qquad(5.32)$$

where $\xi\propto t^{-\nu}$ is the usual correlation length and $\xi_{h_1}\propto h_1^{-\nu/\Delta_1}$ is another characteristic length (McCoy and Wu 1967, Binder and Hohenberg 1972). The total free energy associated with the surface is

$$F_s=\int_0^\infty dz\ (f_s(z)-f_s(\infty))=t^{2-\alpha}\int_0^\infty dz\ (g(z/\xi, z/\xi_{h_1})-1). \tag{5.33}$$

For $\xi_{h_1} \gg \xi$, i.e. $h_1 \ll t^{\Delta_1}$, we set the second argument of g equal to zero and recover equation (5.3). In the limit $t\to 0$ at fixed h_1, however, we have $\xi_{h_1} \ll \xi$. In this limit we set the first argument of g equal to zero to obtain

$$F_s=t^{2-\alpha}\int_0^\infty dz\ (g(0, z/\xi_{h_1})-1) \tag{5.34}$$

$$F_s \propto t^{2-\alpha}\xi_{h_1}. \tag{5.35}$$

To obtain equation (5.35) it was necessary to assume the convergence of the integral in equation (5.34). This is an additional assumption which goes beyond the usual scaling arguments. It is justified by its predictions, which agree with all known exact results.

The singular contributions to the surface magnetisation density m_1 and the local susceptibility $\chi_{1,1}$ are obtained by taking derivatives of equation (5.35) with respect to h_1, evaluated at finite h_1. All such derivatives carry the bulk free-energy density singularity $t^{2-\alpha}$ as $t\to 0$, as anticipated by the mean-field calculation of § 2. Therefore, the surface gap exponent for the extraordinary transition is $\Delta_1^e=0$. Scaling laws for the extraordinary transition are obtained by writing the surface free energy in the form of equation (5.1) (with h a bulk field parallel to the surface magnetisation), but with $\alpha_s=\alpha$ and $\Delta_1^e=0$. The analogues of equations (5.7)–(5.9) are

$$\beta_1^e=2-\alpha \tag{5.36}$$

$$\beta_1^e+\gamma_{1,1}^e=0 \tag{5.37}$$

$$2\gamma_1^e-\gamma_{1,1}^e=\gamma \tag{5.38}$$

where the γ^e are longitudinal susceptibility exponents. Similarly, by writing the longitudinal spin–spin correlation function in scaling form, one obtains the analogues of equations (5.10), (5.12) and (5.13):

$$\gamma_1^e=\nu(2-\eta_\perp^{e,L}) \tag{5.39}$$

$$\eta_\parallel^{e,L}=2\eta_\perp^{e,L}-\eta \tag{5.40}$$

$$\beta_1^e=(\nu/2)(d-2+\eta_\parallel^{e,L}). \tag{5.41}$$

From these scaling laws one deduces the exponent values

$$\gamma_{1,1}^e=\alpha-2 \tag{5.42}$$

$$\gamma_1^e=-\beta \tag{5.43}$$

$$\eta_\parallel^{e,L}=d+2 \tag{5.44}$$

$$\eta_\perp^{e,L}=\tfrac{1}{2}(d+2+\eta). \tag{5.45}$$

Note that the analogue of equation (5.11), $\gamma_{1,1}^e=\nu(1-\eta_\parallel^{e,L})$ would imply $\gamma_{1,1}^e=-\nu(d+1)=\alpha-2-\nu$, a weaker singularity than the true result $\gamma_{1,1}^e=\alpha-2$. Such a term is presumably present as a correction to scaling, but does not provide the dominant singularity.

For $d=4$, equations (5.36) and (5.42) give $\beta_1^e = 2 = -\gamma_{1,1}^e$, in agreement with the mean-field results of § 2, while equations (5.44) and (5.45) give $\eta_\parallel^{e,L} = 6$ and $\eta_\perp^{e,L} = 3$ in agreement with the mean-field calculations of LR. An additional check is provided by the two-dimensional Ising model (McCoy and Wu 1967) which has $\eta_\parallel^e = 4$, in agreement with equation (5.44).

Finally we discuss the exponents associated with the transverse spin–spin correlation function.

Consider the following situation in which there is an infinitesimal bulk field h and in addition a small transverse field h_1^T in the surface. For an infinite system Brézin and Wallace (1973) have shown that for $t<0$ the transverse components of the field variables have their canonical scaling dimensions $(d-2)/2$. This means that the transverse magnetisation $m^T(z)$ set up by the transverse surface field will fall off with distance from the surface as $z^{-(d-2)/2}$. But

$$m^T(z) = \hat{G}_{k=0}^T(z, 0) h_1^T \tag{5.46}$$

which implies that $\hat{G}_{k=0}^T(z, 0)$ should vary with z as $z^{-(d-2)/2}$. The z dependence of $\hat{G}_k^T(z, 0)$ can be expressed in terms of $\eta_\parallel^{e,T}$, but it is easier to recognise that the result for the correlation function in the large n limit already has the correct z dependence. Hence the results given in equations (3.53) and (3.54), namely $\eta_\parallel^{e,T} = d$, $\eta_\perp^{e,T} = d/2$ are almost certainly valid outside the large n limit. Notice that the scaling relation $2\eta_\perp = \eta_\parallel + \eta$ does not directly apply to the transverse exponents unless one recognises that η for transverse correlations is effectively zero as the transverse field components have their canonical dimensions.

6. Discussion

The exact exponent results for the ordinary and extraordinary transition are summarised in table 1. These exponent values agree with all known exact results, namely, the two-dimensional Ising model, the ϵ expansion to $O(\epsilon)$ and the $n=\infty$ limit. We exclude the spherical models discussed in the literature, since they are unphysical for reasons given earlier. We have been unable to find scaling arguments which give the exponents for the special transition. In table 2, the exponents for this transition are

Table 1. Exact exponents for the ordinary and extraordinary transitions. In the right-hand column, (L) and (T) refer to longitudinal and transverse correlations respectively. The exponents for the surface transition are those of the $(d-1)$-dimensional bulk system.

Exponent \ Transition	Ordinary	Extraordinary
$\gamma_{1,1}$	$\nu - 1$	$\alpha - 2$
γ_1	$\nu + (\gamma - 1)/2$	$-\beta$
β_1	$\frac{1}{2} + \nu(d-2)/2$	$2 - \alpha$
Δ_1	$(1-\alpha)/2$	0
$\eta_\parallel$	$1/\nu$	(L) $d+2$
		(T) d
$\eta_\perp$	$1 - (\gamma - 1)/2\nu$	(L) $(d+2+\eta)/2$
		(T) $d/2$

Table 2. Critical exponents for the special transition to $O(\epsilon)$ and for $n=\infty$. The results for $\eta_\parallel$ were derived in the text, the other results obtained from the scaling laws (5.7)–(5.13).

Exponent	$O(\epsilon)$	$n=\infty$
$\gamma_{1,1}^{sp}$	$\frac{1}{2}+3\epsilon(n+2)/4(n+8)$	$(5-d)/(d-2)$
γ_1^{sp}	$1+3\epsilon(n+2)/4(n+8)$	$(8-d)/2(d-2)$
β_1^{sp}	$\frac{1}{2}-\epsilon/4$	$(d-3)/(d-2)$
Δ_1^{sp}	$1+\epsilon(n-1)/2(n+8)$	$2/(d-2)$
$\eta_\parallel^{sp}$	$-\epsilon(n+2)/(n+8)$	$d-4$
$\eta_\perp^{sp}$	$-\epsilon(n+2)/2(n+8)$	$(d-4)/2$

given to $O(\epsilon)$ and for $n=\infty$. The scaling laws, (5.7)–(5.13), have been used to derive all the exponent values from those for $\eta_\parallel$ given earlier.

All four transitions may be observed in the c–t plot of figure 7, which is a section of the phase diagram with $h_1=0=h$. The ordinary transition corresponds to crossing the line $t=0$ above the point P, which is the point $c=0$ for the infinite system and the point $c=c^*$ for the semi-infinite system. The bulk (or special) transition corresponds to crossing the line $t=0$ at the point P for the infinite (or semi-infinite) system. The surface transition corresponds to crossing the line PQ and the extraordinary transition to crossing the line $t=0$ below the point P. The extraordinary transition may also be observed in the h_1–t plot of figure 8, which is a section of the phase diagram with c constant and $h=0$. The extraordinary transition corresponds to crossing the line $t=0$ at any $h_1\neq 0$, regardless of the value of c. The nature of the transition for $h_1=0$ depends on the value of c according to figure 7.

The nature of the phase diagram, figure 7, when the surface transition does not occur (i.e. when the $(d-1)$-dimensional system has no phase transition) is an interesting problem. For the infinite system the point P remains fixed at $c=0$, corresponding

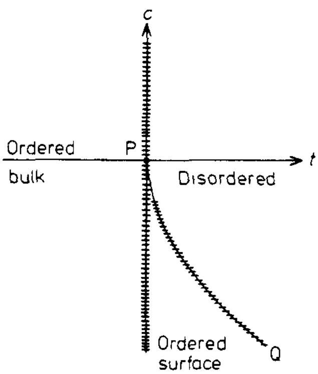

Figure 7. Phase diagram as a function of c and t for $h_1=0=h$. P is the point $c=0$ for the infinite problem and $c=c^*$ for the semi-infinite problem. The shape of the line PQ near P is $c\sim t^{1-\nu}$ or $c-c^*\sim t^{1-\nu}$ for infinite and semi-infinite problems respectively. Cross-hatched lines represent phase boundaries as described in the text.

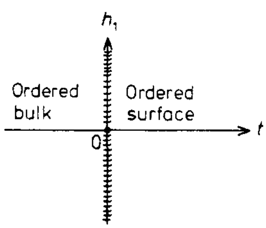

Figure 8. Phase diagram as a function of h_1 and t for c constant and $h=0$. The extraordinary transition corresponds to crossing the line $t=0$ (cross-hatched) at any $h_1\neq 0$.

to the bulk transition, but the line PQ disappears. We conjecture that, provided $\nu < 1$, crossing the line $t = 0$ at any $c \neq 0$ corresponds to the ordinary transition. For $\nu > 1$, of course, crossing the line $t = 0$ at any finite c corresponds to the bulk transition. For the semi-infinite system we conjecture that $c^* \to -\infty$ as $d \to d_c(n)$, the critical dimensionality for splitting off a surface phase, and that the point P is located at $c = -\infty$ if there is no surface phase. Crossing the line $t = 0$ then corresponds to the ordinary transition for any finite value of c.

In addition to the exact results referred to above, there are high-temperature series expansions, low-temperatuture series expansions, Monte Carlo analyses, and one experiment with which we may compare our predictions.

High-temperature series expansions for the semi-infinite three-dimensional Ising model have been performed by Binder and Hohenberg (1972, 1974). These authors found that the values of the exponents appear to depend continuously on the value of the exchange enhancement parameter Δ (recall that the exchange interaction between spins in the surface is $J(1+\Delta)$). For $\Delta < \Delta_c \sim 0{\cdot}6$, the transition occurs at the bulk T_c (the ordinary transition), with an 'effective exponent' γ_1^{eff} which increases from $\gamma_1^{\text{eff}} \sim 0{\cdot}75$ at $\Delta = -0{\cdot}2$ to $\gamma_1^{\text{eff}} \sim 1{\cdot}65$ at $\Delta = 0{\cdot}6$. For $\Delta > \Delta_c$ the transition occurs at a higher temperature (the surface transition) with $\gamma_1 = \gamma_{2d} = 7/4$, the susceptibility exponent for the $d = 2$ Ising model. Similar results were obtained for the exponent $\gamma_{1,1}$. Binder and Hohenberg (1974) identified the apparent variation of the exponents for $\Delta < \Delta_c$ as an artefact of their rather short series, which sample the 'crossover' from the ordinary to the surface transition. We agree with this diagnosis, but believe that the crossover seen by the series expressions is between the ordinary and special transitions, since $\Delta = \Delta_c$ is just that value of the exchange enhancement appropriate to the special transition. The mechanism of the crossover may be seen in equation (5.22). For this asymptotic form to hold one requires $t^{-\gamma_{1,1}} = t^{1-\nu} \ll c$. In the opposite regime $t^{1-\nu} \gg c$ (or $t^{1-\nu} \gg c - c^*$) the critical behaviour is dominated by the bulk (or special) critical exponents for the infinite (or semi-infinite) system. We conclude that no reliable values for the ordinary exponents can be extracted from the series data. In particular, we do not feel that Binder and Hohenberg's estimate $\gamma_1 \sim 7/8$ obtained with $\Delta = 0$ (since this choice of Δ gave the least curvature in the ratio plot) can be taken as contradicting our prediction $\gamma_1 = \nu + (\gamma - 1)/2 \sim 3/4$.

Low-temperature series expansions have been performed by Barber (1973b) who obtained $\beta_1 = 0{\cdot}72 \pm 0{\cdot}03$ for the FCC lattice. Our prediction is $\beta_1 = \frac{1}{2} + \nu(d-2)/2 \sim 0{\cdot}82$. Low-temperature series, however, are often quite unreliable even for the bulk, since they often show seemingly spurious lattice dependences (Domb and Guttman 1970). In addition, crossover effects may also play an important role here.

Binder and Hohenberg (1974) have performed a Monte Carlo study of finite Ising films with periodic boundary conditions on the four sides, and free boundary conditions on the other two ends. The results are again very sensitive to the value of Δ with $\beta_1^{\text{eff}} = 0{\cdot}66$ for $\Delta = 0$ and $\beta_1^{\text{eff}} = 0{\cdot}86$ for $\Delta = -0{\cdot}5$. We believe that no reliable conclusions can be drawn.

The one experiment to be performed so far is a measurement of β_1 for NiO using LEED (Wolfram *et al* 1971). For the Heisenberg model, with $\nu \simeq 0{\cdot}7$, we predict $\beta_1 \simeq 0{\cdot}85$. The experimental data are consistent with $\beta_1 = 1$, but it is not clear that the data are sufficiently precise to distinguish between exponent values of unity and 0·85. Further experiments are clearly desirable. The exponent β_1 would seem to be the most accessible experimentally, using a local probe such as LEED or the Mössbauer effect. With regard to the latter technique it has, to our knowledge, not yet been demonstrated that the local magnetisation in the neighbourhood of the Mössbauer impurity has the same critical behaviour as the magnetisation far from the impurity. That this is so is readily proved if the impurity is represented by a term in the Hamiltonian similar to that which represents the surface in equation (5.15):

$$H_{\mathrm{I}} = \tfrac{1}{2} g \int \mathrm{d}^d x \, \delta(\boldsymbol{x}) \sum_{i=1}^{n} \phi_i^2(\boldsymbol{x}) \tag{6.1}$$

where we have located the impurity at $\boldsymbol{x} = 0$ and the δ-function is d-dimensional so that the impurity is a point defect. Under a scale transformation g is rescaled in a fashion analogous to the rescaling of c in equation (5.17), namely

$$g' = b^{-(1-\alpha)/\nu} g. \tag{6.2}$$

Provided $\alpha < 1$ (which is always the case in practice) the perturbation H_{I} is an irrelevant operator, and the Mössbauer effect may be used with full confidence that of severe crossover problems, so that the extant calculations do not provide reliable values for the exponents. Similar crossover problems may complicate the interpretation of experimental data.

Acknowledgment

The authors wish to thank Dr Paul Reed for numerous helpful discussions concerning the critical behaviour of the semi-infinite two-dimensional Ising model.

Appendix

We wish to evaluate the integral

$$I=\int_0^\infty \mathrm{d}t\, t^{d-3}(tI_\mu(t)K_\mu(t)-\tfrac{1}{2}).$$

Since the two contributions do not separately converge, it is convenient to write

$$I=\lim_{\epsilon\to 0}\int_0^\infty \mathrm{d}t\, t^{d-3}\left(tI_\mu(t)K_\mu((1+\epsilon)t)-\frac{\exp(-\epsilon t)}{2(1+\epsilon)^{1/2}}\right). \tag{A.1}$$

The first term is now a convergent integral and gives (Gradshteyn and Ryzhik 1965, p 693, no. 5)

$$I_1=\frac{\Gamma[\frac{1}{2}(d-1)+\mu]\Gamma[\frac{1}{2}(d-1)]}{2^{3-d}\Gamma(\mu+1)(1+\epsilon)^{d-1+\mu}}F\left(\frac{d-1}{2}+\mu,\frac{d-1}{2};\mu+1;(1+\epsilon)^{-2}\right)$$

where $F(\alpha,\beta;\gamma;x)$ is the hypergeometric function. Using one of the transformation formulae for hypergeometric functions (Gradshteyn and Ryzhik 1965, p 1043, equation (9.131) no. 2) we can write I_1 in the form

$$I_1=\frac{\Gamma(2-d)\Gamma[\frac{1}{2}(d-1)]\Gamma[\frac{1}{2}(d-1)+\mu]}{2^{3-d}\Gamma[\frac{1}{2}(3-d)]\Gamma[\frac{1}{2}(3-d)+\mu]}F\left(\frac{d-1}{2}+\mu,\frac{d-1}{2};d-1;1-(1+\epsilon)^{-2}\right)$$
$$+\frac{\Gamma(d-2)}{2^{3-d}[1-(1+\epsilon)^{-2}]^{d-2}(1+\epsilon)^{d-1+\mu}}$$
$$\times F\left(\frac{3-d}{2},\frac{3-d}{2}+\mu;3-d;1-(1+\epsilon)^{-2}\right).$$

The second contribution to equation (A.1) is readily evaluated:

$$I_2=\frac{-\Gamma(d-2)}{2\epsilon^{d-2}(1+\epsilon)^{1/2}}.$$

Adding I_1 and I_2 and taking the limit $\epsilon\to 0$ gives the desired result, equation (3.27).

References

Abe R 1972 *Prog. Theor. Phys.* **48** 1414
—— 1973a *Prog. Theor. Phys.* **49** 113
—— 1973b *Prog. Theor. Phys.* **49** 1877
Abe R and Hikami S 1973 *Phys. Lett.* A **45** 11
Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
Au-Yang H 1973 *J. Math. Phys.* **14** 937
Barber M N 1973a *Phys. Rev.* B **8** 407
—— 1973b *J. Phys. C: Solid St. Phys.* **6** L262
—— 1974 *J. Statist. Phys.* **10** 59
Barber M N, Jasnow D, Singh S and Weiner R A 1974 *J. Phys. C: Solid St. Phys.* **7** 3491
Béal-Monod M T, Kumar P and Suhl H 1972 *Solid St. Commun.* **11** 885
Berlin T H and Kac M 1952 *Phys. Rev.* **86** 821
Binder K 1972 *Physica* **62** 508
Binder K and Hohenberg P C 1972 *Phys. Rev.* B **6** 3461
—— 1974 *Phys. Rev.* **B 9** 2194
Bray A J and Moore M A 1977a *Phys. Rev. Lett.* **38** 735
—— 1977b *Phys. Rev. Lett.* **38** 1046
Brézin E and Wallace D 1973 *Phys. Rev.* B **7** 1967
Case K M 1950 *Phys. Rev.* **80** 797
Domb C and Guttman A J 1970 *J. Phys. C: Solid St. Phys.* **3** 1652
Ferdinand A E and Fisher M E 1969 *Phys. Rev.* **185** 832
Ferrell R A and Scalapino D J 1972a *Phys. Rev. Lett.* **29** 413
—— 1972b *Phys. Lett.* A **41** 371
Fisher M E 1971 *Critical Phenomena* ed. M S Green (New York: Academic) pp 1*ff*
—— 1973 *J. Vac. Sci. Technol.* **10** 665
—— 1974 *Rev. Mod. Phys.* **46** 597
Fisher M E and Barber M N 1972 *Phys. Rev. Lett.* **28** 1516
—— 1973 *Ann. Phys., NY* **77** 1
Fisher M E and Ferdinand A E 1967 *Phys. Rev. Lett.* **19** 169
de Gennes P G 1976 *J. Physique* **37** 1445
Gradshteyn I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York: Academic) p 697
Hikami S 1973 *Prog. Theor. Phys.* **49** 1096
Kaganov M I and Omelyanchouk A M 1971 *Zh. Eksp. Teor. Fiz.* **61** 1679 (1972 *Sov. Phys.-JETP* **34** 895)
Lubensky T C 1975 *Phys. Rev.* B **11** 3573
Lubensky T C and Rubin M H 1973 *Phys. Rev. Lett.* **31** 1469
—— 1975a *Phys. Rev.* B **12** 3885
—— 1975b *Phys. Rev.* B **11** 4533
Ma S 1973a *Rev. Mod. Phys.* **45** 589
—— 1973b *Phys. Rev.* A **7** 2172
McCoy B M and Wu T T 1967 *Phys. Rev.* **162** 436
Mills D L 1971 *Phys. Rev.* B **3** 3887
Singh S, Jasnow D and Barber M N 1975 *J. Phys. C: Solid St. Phys.* **8** 3408
Stanley H E 1968 *Phys. Rev.* **176** 718
Weiner R A, Béal-Monod M T and Mills D L 1973 *Phys. Rev.* B **7** 3399
Wilson K G 1972 *Phys. Rev. Lett.* **28** 548
Wilson K G and Fisher M E 1972 *Phys. Rev. Lett.* **28** 240
Wilson K G and Kogut J 1974 *Phys. Rep.* **12** 77
Wolfram T, de Wames R E, Hall W F and Palmberg P W 1971 *Surface Sci.* **28** 45