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The critical behaviour of the spherical model with layered impurities

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Abstract. We analyse the critical behaviour of a three-dimensional spherical model with nearest-neighbour ferromagnetic interactions (of strength $J>0$) in which there is a regular array of planes of bond defects (perpendicular to the planes) of strength J': $0 \leq J' \leq J$ spaced n lattice sites apart. For a fixed, non-zero defect strength J', the critical temperature has the form $T_c(J', n) = T_c(\text{pure}) + c_1(J')n^{-1} + c_2(J')n^{-2} + o(n^{-2})$. For $J' = 0$ the problem reduces to that of finite size effect, while at $J' = J$ the system becomes homogeneous. Two asymptotically distinct scaling regions correspond to these limiting cases. In both scaling regions the spherical field scales with the variable $x \equiv n^2\phi$ where ϕ is proportional to the deviation in spherical field. In terms of the variable $\lambda \equiv 1-(J'/J)^2$ and its conjugate $\bar{\lambda} = (J'/J)^2$, the impurity strength scales as $y = n\lambda$ in the region near $J' = J(\lambda = 0)$ and as $\bar{\lambda}$ for J' away from zero. These scaling relationships are valid for the spherical constraint equation and the thermodynamic quantities such as the specific heat and entropy.

1. Introduction

The effects of impurities and defects on the critical behaviour of magnetic systems have been studied by many authors (see e.g. Harris 1974, Herman and Dorfman 1968, Lee 1974, McCoy and Wu 1968, Sawada and Osawa 1972, Suzuki 1974, Rapaport 1972a, b, Miyazima 1973, Au-Yang *et al* 1976, Au-Yang 1976, Fisher and Au-Yang 1975). Related problems involving perturbations to critical behaviour are associated with finite size, restricted dimensionality and surfaces (Ferdinand and Fisher 1969, Fisher and Ferdinand 1967, Barber and Fisher 1973, Fisher and Barber 1972). Much previous work on both of these questions involves utilising approximations or numerical techniques whose validity is difficult to establish; however, several extensive exact calculations have been performed on the Ising and spherical models. Among these are (i) work on the specific heat anomaly in an $n \times m$ Ising spin system, and the effects of a surface on critical behaviour, by Fisher and Ferdinand (1967; Ferdinand and Fisher 1969); (ii) the calculations (Au-Yang *et al* 1976, Au-Yang 1976, Fisher and Au-Yang 1975) of the shift in critical temperature and near-critical thermodynamic functions for square lattice Ising models with regular arrays of various types of point defect; (iii) the study of the effect of finite thickness on the critical behaviour of the spherical model (Barber and Fisher 1973); (iv) the work by McCoy and Wu (1968) on a square lattice Ising model with random layered impurities.

In this paper we analyse the critical-point behaviour of a three-dimensional spherical model with nearest-neighbour ferromagnetic interactions (of strength $J>0$) in which there is a regular array of planes of bond defects of strength J': $0 \leq J' \leq J$

(perpendicular to the planes) spaced n lattice sites apart (see figure 1). For $J' \equiv J$ and arbitrary n, or for J' arbitrary and $n \to \infty$, the model reduces to the original uniform or homogeneous three-dimensional model. For a fixed strength of impurity J' the problem is analogous to that studied by Au-Yang, Fisher and Ferdinand (Au-Yang *et al* 1976, Au-Yang 1976, Fisher and Au-Yang 1975). On the other hand, if the full range of J' is considered, the problem involves crossover behaviour from two-dimensional to three-dimensional critical behaviour via two independent parameters, namely J'/J and n. In the spherical model, this is particularly interesting since the two-dimensional system does not exhibit a transition at non-zero temperature, while the three-dimensional system has a phase transition at a finite temperature. In the limit $J' \equiv 0$, where each film of width n is independent of all other films, the problem is completely equivalent to the finite size effect problem in which a d-dimensional system is infinite in $d-1$ dimensions and finite (of length n) in the other dimension.

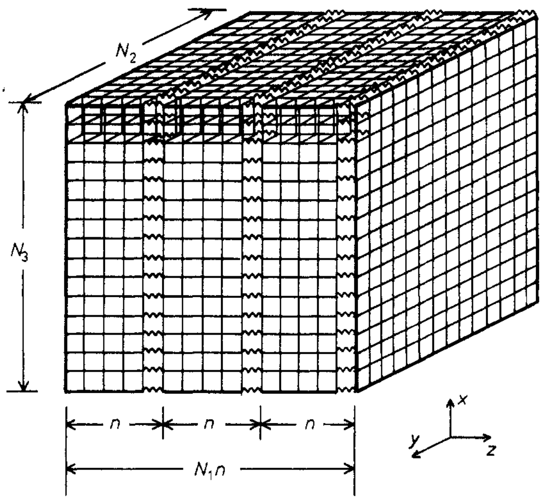


Figure 1. Illustration of a three-dimensional cubic lattice with nearest-neighbour bond interactions J with layers of impurities of bond strength J' in planes, spaced n apart, parallel to the xy plane. The thermodynamic limit is taken by allowing N_1, N_2, N_3, to approach ∞ while n remains fixed. — J; ⁓ J'.

Hence, in the special case $J' \equiv 0$ our explicit results should and do reproduce the corresponding expressions of Barber and Fisher. These results further illuminate the transition from finite size to the full three-dimensional system in that this transition can also be induced by means of the parameter J'/J.

The full range of behaviour of the model in terms of the parameters n $(1 \leq n \leq \infty)$ and

$$\lambda \equiv 1-(J'/J)^2, \qquad \bar{\lambda} = 1-\lambda = (J'/J)^2 \tag{1.1}$$

$(0 \leq \lambda \leq 1)$ is illustrated in figure 2. One of the interesting questions is whether the transitions from various limiting parts of this diagram are described continuously by one scaling relationship, or whether, for example, the region $\lambda = 0$ is asymptotically completely separated from the $\lambda = 1$ region. In fact we find that the scaling variables differ in the two regions, i.e. near $\lambda = 0$ and $\lambda = 1$, while the transition between the two regimes is accomplished smoothly by means of a function involving the scaling variables

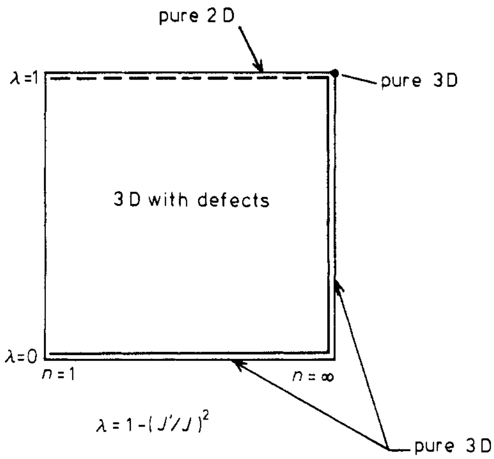


Figure 2. Schematic representation of the impurity problem in terms of the parameters λ, which is a measure of impurity strength, and n, which is a measure of concentration. For $\lambda = 0$ (i.e. $J' = J$) and arbitrary n one has no impurities, represented by the lower horizontal line; for $n = \infty$ and arbitrary λ, one also has pure three-dimensional behaviour, represented by the vertical line on the right. In the case of $\lambda = 1$, the lattice decouples and becomes a set of independent two-dimensional systems as indicated by the upper horizontal line.

of both regions. The scaled variable involving the reduced spherical field z and its critical value z_c (see (4.3) and the Appendix) is found to be

$$x = n^2\phi \qquad (\phi \equiv z - z_c) \tag{1.2}$$

and is valid throughout the entire λ-region. The scaled variable involving λ differs in the two regimes mentioned above; near $\lambda = 0$ the scaled variable is

$$y = n\lambda, \tag{1.3}$$

while at the $\lambda = 1$ end the scaled variable is simply $\bar{\lambda}$. Thus, with $K \equiv J/k_B T$, where T is temperature, the spherical constraint equation (see (2.12)) may be expressed in the form (with the omission of minor corrections to scaling)

$$2K \approx W_3(z) + n^{-1} f(x, y, \bar{\lambda}) \tag{1.4}$$

for large n and arbitrary λ, where the first term on the right-hand side is the expression for the homogeneous model. In the region $\lambda \sim 0$, the variable $\bar{\lambda}$ is unnecessary as a scaling variable, while for $\lambda \gg n^{-1}$, x does not play a role in the scaling behaviour.

The scaling behaviour of the spherical constraint equation governs the thermodynamic functions. The expression (1.4) implies, for example, that the zero-field specific heat per spin, $C_H(T)$, has the form (see (7.11) and (7.12))

$$C_H(T) \approx C_H(\text{pure}, T) + n^{-1} 2J^2/k_B T^2 [\partial f(x, y, \bar{\lambda})/\partial \phi]_S \tag{1.5}$$

where the subscript S indicates that the parameter ϕ is determined by the spherical constraint (1.4). Thus, the behaviour in the two regions of λ and the crossover between these regimes as discussed above applies to the specific heat as well. Thermodynamic functions such as the entropy and internal energy are obtainable in a similar way.

In addition to the scaling relationships we also obtain an asymptotic expression for the critical temperature $T_c(\lambda, n)$. For fixed, non-zero λ, we find that as $n \to \infty$ the critical temperature is of the form

$$T_c(\lambda, n) = T_c(0) + c_1(\lambda)n^{-1} + c_2(\lambda)n^{-2} + o(n^{-2}). \quad (1.6)$$

This is to be compared with the work of Au-Yang, Fisher and Ferdinand in which the critical shift for a two-dimensional Ising model with regularly spaced point impurities of concentration $1/n$ entails a term of the form $n^{-2} \ln n$. The scaling theory advanced by Fisher and Au-Yang (1975) traces the origin of the $n^{-2} \ln n$ term to the logarithmic divergence of the specific heat. In a qualitative sense, our results are consistent with this scaling hypothesis since the spherical model does not exhibit any specific heat divergence and the corresponding argument would at worst suggest a $n^{-3} \ln n$ term. However, it should be emphasised that planes of impurities could well influence the critical behaviour in a way which is rather different from point defects.

The main part of our analysis concerns the spherical constraint equation (see equation (2.12)), which essentially governs the overall thermodynamic behaviour of the model. The critical temperature is obtained quite directly (see § 2) from this equation.

Specifically, the contents of the subsequent sections are as follows. In § 2, we begin by defining the spherical model in the mean spherical form and discussing some of the essential features of the pure two- and three-dimensional models. The problem of layered impurities is then formulated and the fundamental parameters are defined. In § 3, the matrix $(s\boldsymbol{I} - \boldsymbol{J})$ for a finite system, where s is the spherical field, $\boldsymbol{I}$ is the identity matrix while $\boldsymbol{J}$ is the matrix of interactions (including impurities), is transformed and its determinant is evaluated as a three-fold product. In § 4, the logarithm of this determinant is analysed in the thermodynamic limit of infinite system size for fixed n. An expression is obtained in which the temperature is expressed in terms of the generalised Watson function (Barber and Fisher 1973) $W_3(z)$ and two double integrals which are analysed in subsequent sections. At this point we consider different scaling regimes separately. First, in § 5, the situations for J' fixed with $J' \neq J$ and $J' \to 0$ are analysed, and an asymptotic expression for the shift in critical temperature is obtained for J' fixed. In § 6, the situation for $J' \to J$ (as $n \to \infty$) is analysed and the crossover behaviour between this limit and the J' fixed and $J' \to 0$ limits is described explicitly. A qualitative discussion of the crossover behaviour and the implications for various thermodynamic functions is the topic of § 7. In § 8, we discuss the formulation of the problem for other dimensions and co-dimensions (i.e. dimensionality of space minus dimensionality of impurities).

2. Formulation of the problem

The spherical model of a ferromagnet was originally proposed by Kac, and later solved exactly by Berlin and Kac (1952; Joyce 1972). The rigid 'constraint'

$$\sigma_i^2 = 1 \quad (2.1)$$

which is satisfied by each of the spin variables $\sigma_i = \pm 1$ at the ith site of an Ising model lattice is relaxed and replaced with the overall 'spherical constraint'

$$S^2 \equiv \sum_{i=1}^{N} \sigma_i^2 = N \quad (2.2)$$

where the σ_i: $-\infty<\sigma_i<\infty$ are now taken as continuous real variables. In the thermodynamic limit (in which $N\to\infty$) the strict spherical constraint (2.2) may be replaced with no error by the 'mean spherical constraint'

$$\left\langle N^{-1}\sum_{i=1}^{N}\sigma_i^2\right\rangle=1 \tag{2.3}$$

where $\langle\cdot\rangle$ denotes the standard expectation value or ensemble average,

$$\langle X\rangle\equiv\mathrm{Tr}(X\,\mathrm{e}^{-\beta\mathcal{H}})/\,\mathrm{Tr}(\mathrm{e}^{-\beta\mathcal{H}})\qquad(\beta\equiv 1/k_{\mathrm{B}}T).$$

The mean spherical constraint (2.3) may be expressed in a more convenient form by introducing a spherical field $-s$, conjugate to S^2, directly into the partition function. The Hamiltonian for the so-called mean spherical model is then

$$\mathcal{H}=-\sum_{(i,j)}J_{ij}\sigma_i\sigma_j-\sum_{i=1}^{N}h_i\sigma_i+s\sum_{i=1}^{N}\sigma_i^2, \tag{2.4}$$

where we assume the lattice of N sites is a section of a d-dimensional hypercubic lattice (although more general lattices may be considered without introducing further difficulties). The parameters J_{ij} are the exchange energies between spins at sites i and j, while $h_i=mH_i$ is the (reduced) magnetic field at site i. The first sum in (2.4) runs over all pairs of spins. The partition function and free energy per spin are then given by

$$Z_N=\int_{-\infty}^{\infty}\mathrm{d}\sigma_1\ldots\int_{-\infty}^{\infty}\mathrm{d}\sigma_N\,\exp[-\beta\mathcal{H}(\sigma_1,\ldots,\sigma_N)], \tag{2.5}$$

$$F(\beta,\{h_i\},s)=-(1/\beta N)\ln Z_N(\beta,\{h_i\},s). \tag{2.6}$$

The mean spherical constraint (2.3) may now be written in terms of the free energy as

$$\langle\mathrm{S}^2/N\rangle=(\partial/\partial s)F(\beta,\{h_i\},s)=1. \tag{2.7}$$

The first term in the Hamiltonian (2.4) is a symmetric quadratic form in the spin variables. Hence, it is diagonalised by an $N\times N$ unitary matrix $\boldsymbol{U}$ which must satisfy

$$\boldsymbol{UJU}^{-1}=\boldsymbol{D}, \tag{2.8}$$

where $\boldsymbol{J}=\{\tfrac{1}{2}J_{ij}\}$ is the interaction matrix and $\boldsymbol{D}$ is the diagonal matrix $\boldsymbol{D}_{pq}=\delta_{pq}\mu_q$ while μ_q $(q=0,\ldots,N-1)$ are the eigenvalues of $\boldsymbol{J}$ in decreasing order. Upon defining the variables ϵ_q by

$$\epsilon_q=\sum_{i=1}^{N}U_{qi}, \tag{2.9}$$

and restricting the fields to be uniform $(h_i\equiv h)$, the free energy may be written as

$$F(\beta,h,s)=\frac{k_{\mathrm{B}}T}{2N}\sum_{q=0}^{N-1}\ln[\beta(s-\mu_q)]-\frac{h^2}{4N}\sum_{q=0}^{N-1}\frac{|\epsilon_q|^2}{s-\mu_q} \tag{2.10}$$

and the spherical constraint (2.7) is expressed by

$$\frac{1}{2N}\sum_{q=0}^{N-1}\frac{1}{s-\mu_q}=\frac{1}{k_{\mathrm{B}}T}\left(1-\frac{h^2}{4N}\sum_{q=0}^{N-1}\frac{|\epsilon_q|^2}{(s-\mu_q)^2}\right). \tag{2.11}$$

The magnetisation per spin $M(\beta,h)$, the (reduced) zero-field susceptibility $\chi_0(T)$, the entropy per spin $S(\beta,h)$ and the zero-field specific heat per spin $C_H(T)$ can now be expressed in the following form:

$$M(\beta, h) = -\left(\frac{\partial F}{\partial H}\right)_{\beta,s} = \frac{h}{2N} \sum_{q=0}^{N-1} \frac{|\epsilon_q|^2}{s-\mu_q}, \qquad (2.12)$$

$$\chi_0(T) = \lim_{H\to 0} (\partial M/\partial H)_{T,S} = \lim_{h\to 0} [M(\beta, h)/h], \qquad (2.13)$$

$$S(\beta, h) = -(\partial F/\partial T)_{h,s} = \tfrac{1}{2}k_B - (k_B/2N) \sum_{q=0}^{N-1} \ln[\beta(s-\mu_q)], \qquad (2.14)$$

$$C_H(T) = \lim_{H\to 0} T(\partial S/\partial T)_{H,S} = \tfrac{1}{2}k_B - (\partial S/\partial T)_{h=0,S}. \qquad (2.15)$$

Note that the thermodynamic formulae are defined so that they are consistent with those of the original Kac spherical model in the thermodynamic limit.

We will return to these thermodynamic functions toward the end of our analysis (see § 7). At present, however, we concentrate on the spherical constraint equation (2.11) in zero field. Before introducing any inhomogeneities into the lattice, it will be useful to discuss the behaviour of the spherical constraint equation for a pure homogeneous system in the thermodynamic limit ($N\to\infty$). We consider nearest-neighbour ferromagnetic interactions of strength $J>0$ and define the dimensionless inverse temperature

$$K = \beta J = J/k_B T \qquad (2.16)$$

and the reduced spherical field

$$\phi = (s-\mu_0)/J. \qquad (2.17)$$

For such a system in the thermodynamic limit one can show (Barber and Fisher 1973) that the spherical constraint in zero field becomes

$$2K = W_d(\phi), \qquad (2.18)$$

where the generalised Watson function of order d is defined by

$$W_d(\phi) = (2\pi)^{-d} \int_0^{2\pi} \ldots \int_0^{2\pi} \frac{d\theta \ldots d\theta_d}{\phi + 2\sum_{j=1}^{d}(1-\cos\theta_j)}. \qquad (2.19)$$

The analytic properties of these functions have been studied extensively (see Appendix A in Barber and Fisher (1973) for $d=2$ and $d=3$). The critical value of ϕ is $\phi_c = 0$, which determines the critical temperature T_c (at which point the susceptibility diverges) via

$$2K_c = W_d(0). \qquad (2.20)$$

For $d\leqslant 2$ the integral diverges, so $T_c = 0$, while for $d=3$ the integral is finite and may be expressed in terms of complete elliptic integrals of the first kind (Barber and Fisher 1973, Watson 1939), with the result

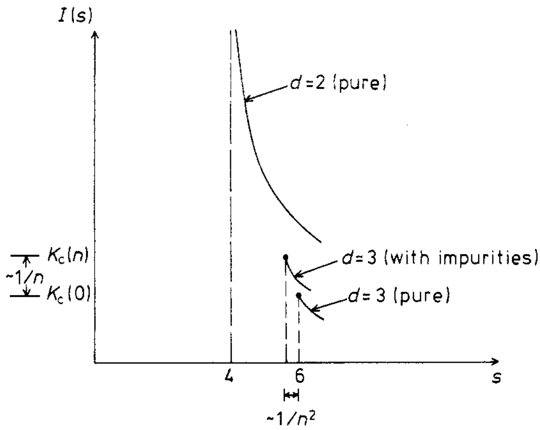
$$K_c(d=3) = 0{\cdot}126\,365\ldots. \qquad (2.21)$$

The behaviour of $W_d(x)$ for small x, which is important in studying the critical region, is

$$W_2(x) = \ln x^{-1}/4\pi + 5 \ln 2/4\pi + x \ln x^{-1}/32\pi + O(x), \tag{2.22}$$

$$W_3(x) = W_3(0) - x^{1/2}/4\pi + O(x) \tag{2.23}$$

for $d = 2$ and $d = 3$ respectively (see figure 3).



$$I(s) = \lim_{N\to\infty} \frac{1}{2N} \sum_{q=0}^{N-1} (s-\mu_q)^{-1}$$

Figure 3. Sketch of the spherical constraint function $I(s)$ for (i) $d = 2$ (pure), for which $I(s)$ is the Watson function in two dimensions W_2, showing the logarithmic divergence at $s = 4$; (ii) $d = 3$ (pure), for which $I(s)$ is the Watson function in three dimensions, W_3, and has a singularity at $s = 6$, $I(s) = W_3(0)$ of the form $(s-6)^{1/2}/4\pi$; (iii) $d = 3$ with impurities, for which $I(s)$ has a singularity of the form $(s-s_c)^{1/2}$ at a critical value s_c which is shifted to the left of $s = 6$ by an amount of the order n^{-2}, corresponding to a shift in K_c of order n^{-1}.

We note also that the functions $W_d(\phi)$ may be generalised to non-integral d, thereby defining a spherical model for non-integral dimension. This device is often useful in determining the origin and behaviour of singularities in thermodynamic functions. We will address this point upon completion of our analysis of two-dimensional layers in three dimensions.

Consider now the spherical constraint (2.11) for an arbitrary matrix $\boldsymbol{J}$. In order to avoid the necessity of determining all of the eigenvalues μ_q, we write the spherical constraint in zero-field as

$$\frac{1}{2N}\frac{\partial}{\partial s} \ln \det(s\boldsymbol{I} - \boldsymbol{J}) = \frac{1}{k_B T}. \tag{2.24}$$

Consequently, an analysis of the determinant of the matrix $(s\boldsymbol{I} - \boldsymbol{J})$ and its largest eigenvalue will be sufficient to determine the critical temperature and the scaling relationships in the critical region.

Let us specialise now to the problem of two-dimensional layers of impurities in a three-dimensional lattice with periodic boundary conditions. Consider a lattice of dimensions N_3, N_2 and $N_1 n$ in the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions (unit vectors $\hat{x}_0$, $\hat{y}_0$, $\hat{z}_0$), respectively, so that $N \equiv N_1 N_2 N_3 n$. The interactions consist of nearest-neighbour ferromagnetic couplings of strength J, except for those bonds which are in the $\hat{z}$ direction and are a distance of a multiple of n away from the xy plane crossing the origin, in which case the interaction is modified to J' (see figure 1). More formally, if A is the set of nearest-neighbour pairs (i, j) and $B = \{(i, j) \in A: i = p\hat{x}_0 + q\hat{y}_0 + rn\hat{z}_0,\ j = p\hat{x}_0 + q\hat{y}_0 + (rn+1)\hat{z}_0\}$ where p, q, r are integers, then the interaction J_{ij} may be defined by

$$J_{ij} = \begin{cases} J & \text{if } (i,j) \in A \backslash B \\ J' & \text{if } (i,j) \in B \\ 0 & \text{otherwise.} \end{cases} \tag{2.25}$$

Let us consider the various limits of these impurities. For $J' = J (\lambda = 0, \bar{\lambda} = 1)$ and arbitrary spacing n between planes of impurities, we recover the pure three-dimensional system. For $J' = 0$ ($\lambda = 1, \bar{\lambda} = 0$) and finite n, we have a set of decoupled, essentially two-dimensional systems (more precisely, each independent system is one of finite thickness, n, in one dimension and infinite in the other two, thereby having two-dimensional critical behaviour at a shifted critical value, s_c, of the spherical field). For infinite layer spacing n, the pure three-dimensional behaviour is once again recovered for arbitrary J'. The situation is represented diagrammatically in figure 2. In between these limiting values of λ and n is a region of a three-dimensional system with impurities. The questions we raise deal with (i) how the critical temperature (and other thermodynamic properties) is shifted for a fixed concentration (in terms of λ and n) of impurities, and (ii) how the various parameters λ, $\bar{\lambda}$, n, ϕ, T_c are scaled in order to produce the transition from two-dimensional behaviour to three-dimensional; in particular, how large n must be in comparison with λ as $\lambda \to 0$, or as $T \to T_c$, etc.

3. The determinant of $(s\boldsymbol{I} - \boldsymbol{J})$

In this section we begin our analysis of equation (2.24) by deriving an identity for $\det(s\boldsymbol{I} - \boldsymbol{J})$. The matrix $s\boldsymbol{I} - \boldsymbol{J}$ may be written in blocks of $N_1 N_2 n$ as

$$s\boldsymbol{I} - \boldsymbol{J} = \begin{pmatrix} E_0 & E_1 & & & E_1 \\ E_1 & E_0 & & & \\ & & \ddots & & \\ & & & E_0 & E_1 \\ E_1 & & & E_1 & E_0 \end{pmatrix} \tag{3.1}$$

where E_0 is the matrix of interactions within individual yz planes and E_1 is the matrix of interactions for neighbouring planes; an explicit definition of E_0 and E_1 will follow. A block cyclic transformation (Camp 1971, Muir 1960) for the matrix (3.1) along the $\hat{x}$ direction yields

$$\det(s\boldsymbol{I} - \boldsymbol{J}) = \prod_{j=1}^{N_3} \det(E_0 + 2\alpha_j E_1) \tag{3.2}$$

with $\alpha_j \equiv \cos(2\pi j/N_3)$.

Similarly, E_0 and E_1 are expressed in blocks of $N_1 n$ as

$$E_0=\begin{pmatrix} B_0 & B_1 & & & & B_1 \\ B_1 & B_0 & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & B_0 & B_1 \\ B_1 & & & & B_1 & B_0 \end{pmatrix}, \qquad E_1=\begin{pmatrix} B_1 & & & & \\ & B_1 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \cdot \\ & & & & & B_1 \end{pmatrix} \tag{3.3}$$

where B_0 is the matrix of interaction for individual rows (i.e. spins along the $\hat{z}$ direction) and B_1 is the matrix of interaction between neighbouring rows. Explicitly, B_0 and B_1 are given by

$$B_0=\begin{pmatrix} C_0 & C_1 & & & & C_1^{\dagger} \\ C_1^{\dagger} & C_0 & C_1 & & & \\ & C_1^{\mathrm{T}} & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & C_1 \\ C_1 & & & & C_1^{\dagger} & C_0 \end{pmatrix}, \qquad B_1=-J\boldsymbol{I} \tag{3.4}$$

where the $n\times n$ matrices C_0 and C_1 are defined by

$$C_0=\begin{pmatrix} s & -J & & & & \\ -J & s & -J & & & \\ & -J & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & -J \\ & & & & -J & s \end{pmatrix}, \qquad C_1=\begin{pmatrix} & & \\ & & \\ & & \\ -J' & & \end{pmatrix}. \tag{3.5}$$

Performing a cyclic transformation in the y direction results in expressing the determinant as

$$\det(s\boldsymbol{I}-\boldsymbol{J})=\prod_{k=1}^{N_2}\prod_{j=1}^{N_3}\det(B_0+2\alpha_j B_1+2\beta_k B_1) \tag{3.6}$$

where $\beta_k=\cos 2\pi k/N_2$. A final cyclic transformation (Camp 1971, Muir 1960) in the $\hat{z}$ direction (in blocks of N_1) yields the form (with $\gamma_l\equiv 2\pi l/N_3$)

$$\det(s\boldsymbol{I}-\boldsymbol{J})=\prod_{l=1}^{N_1}\prod_{k=1}^{N_2}\prod_{j=2}^{N_3}\det(A_0+C_1\,\mathrm{e}^{-\mathrm{i}\gamma_l}+C_1^{\dagger}\,\mathrm{e}^{\mathrm{i}\gamma_l}), \tag{3.7}$$

in which the $n\times n$ matrix A_0 is defined by

$$A_0=\begin{pmatrix} d(j,k) & -J & & & \\ -J & d(j,k) & & & \\ & & \ddots & & \\ & & & & -J \\ & & & -J & d(j,k) \end{pmatrix}, \qquad d(j,k)\equiv s-2(\alpha_j+\beta_k)J. \tag{3.8}$$

Consequently, the problem reduces to evaluating an $n\times n$ matrix, A_n, of the form

$$A_n=\begin{pmatrix} a & b & & & c_1 \\ b & a & b & & \\ & b & \ddots & & \\ & & & \ddots & b \\ c_2 & & & b & a \end{pmatrix}. \tag{3.9}$$

Using the identity (Gradshteyn and Ryzhik 1965)

$$\prod_{r=1}^{n-1}[x^2-2x\cos(\pi r/n)+1]=(x^{2n}-1)/(x^2-1) \tag{3.10}$$

and the definitions $X_{ab}=(a^2-4b^2)^{1/2}$, $Y_{(\pm)}=\frac{1}{2}(a\pm X_{ab})$, the determinant is expressed as

$$|A_n|=\frac{a}{X_{ab}}(Y^n_{(+)}-Y^n_{(-)})-\frac{(b^2+c_1c_2)}{X_{ab}}(Y^{n-1}_{(+)}-Y^{n-1}_{(-)})+(-1)^{n-1}(c_1+c_2)b^{n-1}, \tag{3.11}$$

upon expansion by cofactors.

The identity (3.11) can be applied to the determinant appearing in (3.7) upon making the definitions

$$a=d(j,k)/J=s/J-2\alpha_j-2\beta_k, \qquad b=-1$$
$$c_1=-\sqrt{\lambda}\exp(\mathrm{i}\gamma_l), \qquad c_2=c_1^\dagger \tag{3.12}$$

$$X=(a^2-4)^{1/2}, \qquad Y_\pm=\tfrac{1}{2}(a\pm X) \tag{3.13}$$

and using the identities

$$Y_\pm\frac{a}{X}-\frac{2}{X}=\pm Y_\pm, \tag{3.14}$$

$$\frac{a}{X}Y^n_\pm\mp\frac{2}{X}Y^{n-1}_\pm=Y^n_\pm. \tag{3.15}$$

The determinant of $s\boldsymbol{I}-\boldsymbol{J}$ is thus written in a convenient form as

$$J^{-n}\det(s\boldsymbol{I}-\boldsymbol{J})=\prod_{j,k,l}\left(Y^n_+ + Y^n_- +\frac{\lambda}{X}(Y^{n-1}_+ - Y^{n-1}_-)-2\sqrt{\lambda}\cos\gamma_l\right) \tag{3.16}$$

where the products range over the same variables as in (3.7).

Two limiting cases in (3.16) are noteworthy: (i) in the pure three-dimensional case (i.e. $J' = J$), the middle term in (3.16) vanishes as the determinant assumes the form

$$J^{-n}\det(s\boldsymbol{I}-\boldsymbol{J}) = \prod_{j,k,l}(Y_+^n + Y_-^n - 2\cos\gamma_l), \tag{3.17}$$

which is equivalent, in the thermodynamic limit, to the right-hand side of (2.19); and (ii) in the decoupled, two-dimensional case (i.e. $J' = 0$), the $\cos\gamma_l$ term vanishes, thereby reducing the triple product (which is to become a triple integral) to a double product (and hence a double integral). An analysis beginning directly with (3.17) reproduces, by different methods, the result of Barber and Fisher (1973 § 4) on free edges. This result will also follow as a consequence of more general relations to be established later. An understanding of the limiting cases above facilitates the decomposition of (3.16) into different components responsible for the behaviour of the model in various regions of the parameters.

4. Simplification of the spherical constraint equation

In the last section, $\det(s\boldsymbol{I}-\boldsymbol{J})$ was written (see (3.16)) as a triple product over the discrete variables l, k, j which range up to N_1, N_2, N_3, respectively. Using this expression in the spherical constraint equation (2.24), and taking the thermodynamic limit ($N_1, N_2, N_3 \to \infty$) while n remains fixed so that the sums become integrals in the canonical way, i.e.

$$N^{-1}\sum_{j=1}^{N} f(\cos 2\pi j/N) \to (2\pi)^{-1}\int_0^{2\pi} f(\theta)\,\mathrm{d}\theta,$$

we obtain

$$2K = n^{-1}(2\pi)^{-3}\iiint_0^{2\pi} \mathrm{d}\theta\,\mathrm{d}\phi\,\mathrm{d}\psi \frac{\partial}{\partial(s/J)}\ln A(\theta,\phi,\psi) \tag{4.1}$$

where the variables α_j, β_k, γ_l have been replaced by θ, ϕ and ψ respectively (by taking the thermodynamic limit) in $\det(s\boldsymbol{I}-\boldsymbol{J})$, in which we isolate

$$A(\theta,\phi,\psi) \equiv Y_+^n + Y_-^n + \frac{\lambda}{X}(Y_+^{n-1} - Y_-^{n-1}) - 2\sqrt{\lambda}\cos\psi. \tag{4.2}$$

The function A can be written in more complicated but more useful form by decomposing it into the components which are responsible for its behaviour in the various limits. Most important among these decompositions is the factoring of Y_+^n which is responsible for the pure three-dimensional behaviour; the reasons for the other decompositions will be clear in the subsequent analysis. First, we make the definitions

$$z = s/J - 6 \tag{4.3}$$

(corresponding to ϕ (2.17) for a pure three-dimensional system)

$$\Delta^2 = z + 4(\sin^2 \theta/2 + \sin^2 \phi/2), \tag{4.4}$$

$$p = 1 + \Delta^2/2, \tag{4.5}$$

$$Y_\lambda = \lambda p + (2-\lambda)(p^2-1)^{1/2}, \tag{4.6}$$

$$Y_\lambda^* = \lambda p - (2-\lambda)(p^2-1)^{1/2}, \tag{4.7}$$

$$\bar{Y}_\lambda = \lambda (p^2-1)^{1/2} + (2-\lambda)p, \tag{4.8}$$

$$\bar{Y}_\lambda^* = \lambda (p^2-1)^{1/2} - (2-\lambda)p. \tag{4.9}$$

(Note that Y_λ and Y_λ^* are generalisations of Y_+ and Y_-, respectively, for the case when the planes are not completely decoupling.) We state the identities

$$Y_- = Y_+^{-1}, \tag{4.10}$$

$$1 + \frac{\lambda}{2Y_+(p^2-1)^{1/2}} = \frac{Y_\lambda}{2(p^2-1)^{1/2}}, \tag{4.11}$$

$$Y_\lambda + Y_\lambda^* = 2\lambda p, \tag{4.12}$$

$$(p^2-1)^{1/2}\bar{Y}_\lambda - pY_\lambda = -\lambda, \tag{4.13}$$

$$Y_\lambda (p^2-1)^{1/2} - p\bar{Y}_\lambda = -(2-\lambda), \tag{4.14}$$

with which A may be written as

$$A(\theta, \phi, \psi) = Y_+^n B(\theta, \phi, \psi), \tag{4.15}$$

where the function B is defined by

$$B = 1 + Y_+^{-2n} + \frac{\lambda}{2(p^2-1)^{1/2} Y_+} - \frac{\lambda Y_+^{-2n+1}}{2(p^2-1)^{1/2}} - 2\sqrt{\lambda}\, Y_+^{-n} \cos \psi. \tag{4.16}$$

Factoring further, one may write

$$B = B_{\mathrm{I}} B_{\mathrm{II}}, \tag{4.17}$$

$$B_{\mathrm{I}} = \frac{Y_\lambda}{2(p^2-1)^{1/2}}, \qquad B_{\mathrm{II}} = 1 - \frac{Y_\lambda^*}{Y_\lambda} Y_+^{-2n} - 4\sqrt{\lambda}\frac{(p^2-1)^{1/2}}{Y_\lambda} Y_+^{-n} \cos \psi. \tag{4.18}$$

This leads to the decomposition

$$\frac{\partial}{\partial z} \ln A = n \frac{\partial Y_+/\partial z}{Y_+} + \frac{\partial B_{\mathrm{I}}/\partial z}{B_{\mathrm{I}}} + \frac{\partial B_{\mathrm{II}}/\partial z}{B_{\mathrm{II}}}. \tag{4.19}$$

The first two terms in (4.19) do not involve the variable ψ, while the third involves ψ through the $\cos \psi$ term in (4.18). The identity

$$\partial Y_+/\partial z = Y_+/2(p^2-1)^{1/2} \tag{4.20}$$

reduces the first term to $(n/2)(p^2-1)^{-1/2}$, while the identity

$$\frac{\partial}{\partial z} \frac{Y_\lambda}{2(p^2-1)^{1/2}} = \frac{-\lambda}{4(p^2-1)^{3/2}} \tag{4.21}$$

simplifies the second term to $-\lambda[2(p^2-1)Y_\lambda]^{-1}$. We substitute (4.19) into the spherical constraint equation (4.1) and perform the integrals in the first term, obtaining

$$W_3(z)=(2\pi)^{-2}\int_0^{2\pi} d\theta\int_0^{2\pi} d\phi\, \tfrac{1}{2}(p^2-1)^{-1/2}. \tag{4.22}$$

In the third term, $n^{-1}(2\pi)^{-3}\iiint d\theta\, d\phi\, d\psi\, B_{\rm II}^{-1}(\partial B_{\rm II}/\partial z)$, the differentiation is postponed as it is possible to integrate over the ψ variable by writing $B_{\rm II}$ in the form

$$B_{\rm II}=F-G\cos\psi, \tag{4.23}$$

$$F\equiv 1-\frac{Y_\lambda^*}{Y_\lambda}Y_+^{-2n},\qquad G=4\sqrt{\lambda}\frac{(p^2-1)^{1/2}}{Y_\lambda}Y_+^{-n}, \tag{4.24}$$

and using the relation

$$\int_0^{2\pi}\frac{F'-G'\cos\psi}{F-G\cos\psi}d\psi=\frac{\partial}{\partial z}\ln[F+(F^2-G^2)^{1/2}], \tag{4.25}$$

where primes denote differentiation with respect to z. Combining these results, we can write the spherical constraint equation (4.1) as

$$2K = W_3(z)+\frac{1}{n}(2\pi)^{-2}\iint_0^{2\pi}\frac{-\lambda}{2(p^2-1)Y_\lambda}d\theta\, d\phi$$

$$+\frac{1}{n}(2\pi)^{-2}\iint_0^{2\pi}\frac{\partial}{\partial z}\ln[F+(F^2-G^2)^{1/2}]\,d\theta\, d\phi. \tag{4.26}$$

Up until this point no estimates have been made, as (4.26) and each of the preceding steps has been an identity. We note that the function $W_3(z)$ is not uniquely defined *a priori* for $0>z>-4d$; however we adopt the convention throughout this analysis that the negative z axis will be approached via the limit $v\to 0$ where $z=u+iv$. These questions are discussed further in § 5. In the next section we analyse the integrals in (4.26), bounding remainder terms by $O(n^{-p})$.

5. The scaling regime of λ bounded away from zero

In analysing the integrals in (4.26) we initially consider the two scaling regimes:

(i) when λ is fixed and non-zero, so that $\lambda \gg 1/n$ eventually as n becomes very large;

(ii) when λ approaches zero at a rate faster than n^{-1}.

We will then discuss the crossover between these two regimes. Case (i) includes the limit $\lambda=1$, which, physically, is the situation where the planes decouple the three-dimensional block into independent slabs of thickness n. As discussed in § 1, this limit involves an essentially two-dimensional system for finite n, so that the inverse critical temperature is infinite. Hence, an analysis of case (i) explicitly displays the transition to the two-dimensional system as $\lambda\to 1$ while n is finite. This complements the Barber and Fisher (1973) work, in which the finite size effect ($\lambda=1$, in our terminology) was examined as a function of n.

The main results of this section are the following.

(i) The shift in critical temperature is calculated explicitly to $O(n^{-2})$ for fixed, non-zero λ (see (5.23)). The inverse critical temperature diverges through a $\ln \bar{\lambda}$ term (for fixed n) as the interactions decouple the system into 'films.'

(ii) An expression is obtained, to $O(n^{-2})$, for the spherical constraint near the critical point. This then allows us to compute the basic thermodynamic functions as discussed in § 7.

(iii) The basic scaling parameters in this region are found to be $\bar{\lambda}$, which is mainly responsible for the transition between two- and three-dimensional behaviour, and $x \equiv n^2\phi$, which is a measure of the proximity to the critical value of the spherical field.

An important feature of the spherical constraint equation in the form (4.26) is that the first term does not involve n, and the second term,

$$n^{-1}I_1 = n^{-1}(2\pi)^{-2}\iint_0^{2\pi} \frac{-\lambda}{2(p^2-1)Y_\lambda}\,d\theta\,d\phi, \tag{5.1}$$

involves n only as a multiplicative factor, while the third term,

$$n^{-1}I_2 = n^{-1}(2\pi)^{-2}\iint_0^{2\pi} \frac{\partial}{\partial z}\ln[F+(F^2-G^2)^{1/2}]\,d\theta\,d\phi, \tag{5.2}$$

entails a more complicated n dependence.

In analysing I_1 we may initially consider z as a complex variable which lies in the upper half plane off the negative real axis. Furthermore, we take all branch cuts for $z^{1/2}$, $\log z$, etc. to be in the lower half plane, away from the negative real line, e.g. at $\theta = 5\pi/4$ where $z = r\,e^{i\theta}$. Upon evaluating I_1 as a function of complex z, we may approach real negative z from above by a continuity argument (either by analytic continuation or by an L^∞ version of the Paley–Weiner theorem (see Rudin 1974 p 264). Similar arguments are needed in analysing various parts of I_2, and we must consistently approach the negative real axis from the same direction, i.e. from above.

We begin our analysis of the spherical constraint equation (4.26) (for case (i): λ fixed) by considering the first integral, I_1. Decomposing the integrand by writing

$$\frac{-\lambda}{2(p^2-1)Y_\lambda} = -\frac{1}{4(p+1)} - \frac{1}{4(p-1)} + \frac{2-\lambda}{\lambda}\,\frac{1}{2(p^2-1)^{1/2}} + \frac{2(\lambda-1)}{\lambda}\,\frac{1}{Y_\lambda} \tag{5.3}$$

and performing the first three integrals results in

$$I_1 = -\tfrac{1}{2}W_2(z) - \tfrac{1}{2}W_2(z+4) + \frac{2-\lambda}{\lambda}W_3(z) + (2\pi)^{-2}\frac{2(\lambda-1)}{\lambda}\iint_0^{2\pi} Y_\lambda^{-1}\,d\theta\,d\phi. \tag{5.4}$$

The last integral in I_1 is, of course, a function of z through Y_λ, which we will write explicitly as $Y_\lambda(z)$ when necessary.

In analysing this part of (5.3) we make a choice of scaling which is motivated by the Appendix. The critical value of z, denoted z_c, is determined through (4.3) by the largest root of $A(\theta = \phi = \psi = 0)$ and is found in the Appendix to be bounded by $0 \geqslant z_c \geqslant -\pi/(n+1)^2$ where the upper and lower bounds are taken on at $\lambda = 0$ (pure) and $\lambda = 1$

(decoupled), respectively. We rewrite the reduced spherical field variable ϕ (see (2.17)) and define the scaling variable x as

$$\phi = z - z_c, \tag{5.5}$$

$$x = n^2\phi. \tag{5.6}$$

The last term in (5.4) can thus be analysed as follows. The region of integration can be divided into the two regions $r^2 = \theta^2 + \phi^2 > n^{-1}$ and $r^2 = \theta^2 + \phi^2 < n^{-1}$. One may easily establish the bounds

$$|Y_\lambda(z)Y_\lambda(0)| \geq \lambda^2, \tag{5.7}$$

$$|Y_\lambda(z) - Y_\lambda(0)| \leq |z|^{1/2}, \tag{5.8}$$

from which follows the estimate

$$n^{-1}\iint_0^{2\pi} |Y_\lambda^{-1}(0) - Y_\lambda^{-1}(z)|\,\mathrm{d}\theta\,\mathrm{d}\phi = \mathrm{O}(xn^{-2}, n^{-2}). \tag{5.9}$$

Hence, this last term in (5.4) does not contribute a non-constant term larger than $\mathrm{O}(xn^{-2}, n^{-2})$. This situation is summarised by writing

$$n^{-1}I_1 = -\tfrac{1}{2}W_2(z) - \tfrac{1}{2}W_2(z+4) + \frac{2-\lambda}{\lambda}W_3(z) + C_\lambda + \mathrm{O}(xn^{-2}, n^{-2}) \tag{5.10}$$

where the constant (in the variables z or x) C_λ is defined by

$$C_\lambda = (2\pi)^{-2}\frac{2(\lambda-1)}{\lambda}\iint_0^{2\pi}\left[\lambda + \frac{\lambda\omega^2}{2} + (2-\lambda)(\omega^2 + \omega^4/4)^{1/2}\right]^{-1}\mathrm{d}\theta\,\mathrm{d}\phi, \tag{5.11}$$

with $\omega^2 \equiv 4(\sin^2\theta/2 + \sin^2\phi/2)$.

We continue by analysing the remaining integral in (4.26),

$$I_2 \equiv (2\pi)^{-2}\iint_0^{2\pi}\frac{\partial}{\partial z}\ln[F + (F^2 - G^2)^{1/2}]\,\mathrm{d}\theta\,\mathrm{d}\phi, \tag{5.12}$$

by employing the following strategy.

(i) We divide the region of integration into $r < (k+1)(\ln n)/n$ and $r > (k+1)(\ln n)/n$, where k is an integer ≥ 6, and show that the outer portion does not contribute to the order of interest.

(ii) Within the inner part of the integral, we bound the difference between the internal I_2 and the corresponding integral in which ω^2 has been replaced by r^2.

(iii) We are able to evaluate this new integral exactly and show that only the lower limit contributes significantly.

Step (i) is a routine estimate obtained by writing $\Delta \geq k(\ln n)/n$ for sufficiently large n, which implies $|Y_+^{-2n}| \leq n^{-2k}$ and similarly for Y_λ, Y_λ^*, etc. From this we derive the bounds $|F'| \leq n^{-2k-4}$, $|G'| \leq n^{-k}$, where primes denote differentiation with respect to z, and observe $F = \mathrm{O}(1)$, thus establishing:

$$I_2 = (2\pi)^{-2}\iint_{r<(k+1)\ln n/n}\frac{\partial}{\partial z}\ln[F + (F^2 - G^2)^{1/2}] + \mathrm{O}(n^{-k}). \tag{5.13}$$

To implement part (ii), we let $f(\theta, \phi)$ denote the integrand while $\tilde{f}(\theta, \phi)$ and $\tilde{\Delta}$ are defined as the functions obtained when ω^2 in $f(\theta, \phi)$ and Δ, respectively, are replaced by r^2. Performing the differentiation explicitly, i.e.

$$f(\theta, \phi) = \frac{F' + (FF' - GG')/(F^2 - G^2)^{1/2}}{F + (F^2 - G^2)^{1/2}} \tag{5.14}$$

and analogously for $\tilde{f}(\theta, \phi)$, one may compare the differences in the terms and write I_2 as

$$n^{-1} I_2 = n^{-1} (2\pi)^{-2} \iint_{r<(k+1)(\ln n)/n} \tilde{f}(\theta, \phi)\, d\theta\, d\phi + O(xn^{-2}, n^{-2}). \tag{5.15}$$

The final step involves evaluating (5.15) as an exact integral. The integrand, $\tilde{f}(\theta. \phi)$, is a function of $r^2 = \theta^2 + \phi^2$ only through $\tilde{\Delta} = (z + r^2)^{1/2}$, thereby allowing a change of variables in the derivative via

$$\frac{\partial}{\partial z} \tilde{f}(\theta, \phi) = \frac{1}{2r} \frac{\partial}{\partial r} \tilde{f}(\theta, \phi). \tag{5.16}$$

Changing the integration variables to polar coordinates results in (with $k = 5$)

$$\begin{aligned} I_2 &= (2\pi)^{-1} \int_0^{6 \ln n} r\, dr \frac{1}{2r} \frac{\partial}{\partial r} \ln[F + (F^2 - G^2)^{1/2}] + O(xn^{-2}, n^{-2}) \\ &= \frac{1}{4\pi} \ln[F + (F^2 - G^2)^{1/2}]_{\tilde{\Delta} = [z + 36(\ln n)/n]^{1/2}} \\ &\quad - \frac{1}{4\pi} \ln[F + (F^2 - G^2)^{1/2}]_{\tilde{\Delta} = z^{1/2}} + O(xn^{-2}, n^{-2}) \end{aligned} \tag{5.17}$$

where the subscript $\tilde{\Delta}$ indicates that Δ is replaced by $\tilde{\Delta}$ in the functions within the brackets. Estimating the upper limit, i.e. the first part of (5.17), by the method leading to (5.13), one obtains

$$\text{Upper limit} = (4\pi)^{-1} \ln 2 + O(n^{-5}). \tag{5.18}$$

Hence, the final expression for the integral is

$$I_2 = (4\pi)^{-1} \ln 2 - (4\pi)^{-1} \ln[F + (F^2 - G^2)^{1/2}]_{\theta = \phi = 0} + O(xn^{-1}, n^{-1}). \tag{5.19}$$

Combining (4.26) with (5.10) and (5.19) we have the spherical constraint equation (for λ fixed) as

$$\begin{aligned} 2K = W_3(z) + \frac{1}{n} \{ &-\tfrac{1}{2} W_2(z) - \tfrac{1}{2} W_2(z+4) + [(2-\lambda)/\lambda] W_3(z) + C_\lambda \\ &+ (4\pi)^{-1} \ln 2 - (4\pi)^{-1} \ln[F + (F^2 - G^2)^{1/2}]_{\theta = \phi = 0} \} + O(xn^{-2}, n^{-2}). \end{aligned} \tag{5.20}$$

This can be simplified further, using the expressions (2.22) and (2.23) for the Watson functions, and the estimate $W_2(z+4) = W_2(4) + O(|z|)$, so that (5.20) becomes:

$$\begin{aligned} 2K = W_3(0) &+ \frac{1}{n} \left(-\frac{3}{8\pi} \ln 2 - \tfrac{1}{2} W_2(4) + \frac{2-\lambda}{\lambda} W_3(0) + \frac{1}{4\pi} \ln \lambda + C_\lambda \right) \\ &- \frac{1}{2\pi} \frac{1}{n} \ln[\sqrt{A_0} + (A_0 + 4\sqrt{\bar{\lambda}})^{1/2}] + O(xn^{-2}, n^{-2}), \end{aligned} \tag{5.21}$$

where A_0 is the function defined by (4.2) and evaluated at $\theta = \phi = \psi = 0$.

For a given λ, z_c can be computed from $A_0 = 0$ (see Appendix) and equation (5.21) can be stated in terms of $\phi = z - z_c$. Much information is obtained from studying equation (5.21) from this perspective; however, we postpone this analysis until § 7, at which point we derive the analogous equation in which λ is also allowed to vary as a scaling parameter.

The (reduced) inverse critical temperature is given by

$$2K_c = W_3(0) + \frac{1}{n}\left(-\frac{7}{8\pi}\ln 2 - \tfrac{1}{2}W_2(4) + \frac{2-\lambda}{\lambda}W_3(0) + \frac{1}{4\pi}\ln(\lambda/\sqrt{\bar{\lambda}}) + C_\lambda\right) + O(xn^{-2}, n^{-2}). \tag{5.22}$$

As expected, the inverse critical temperature for the decoupled system ($\bar{\lambda} = 0$) diverges through the $\ln\sqrt{\bar{\lambda}}$ term. It is also interesting to note that a logarithmic term of the form $n^{-2}\ln n$ is not present in (5.22). Such a term had been observed by Au-Yang *et al* (1976) in their work on the two-dimensional Ising model with regular arrays of point defects (with concentration n^{-1}).

6. Analysis near $\lambda = 0$ and crossover between scaling regimes

In this section we first consider the spherical constraint equation in case (ii), i.e. when $\lambda \to 0$ faster than n^{-1}, and then analyse the crossover behaviour between the scaling regimes of case (i) (λ fixed, non-zero) and case (ii). The scaling parameter which serves as a measure of the relative size of λ in comparison with n^{-1} is found to be

$$y = n\lambda. \tag{6.1}$$

An expression for the spherical constraint in case (ii) is obtained (see (6.9)). The behaviour of the spherical constraint in the crossover between the scaling regimes of λ fixed, non-zero and $\lambda \to 0$ is accomplished largely through a rather complicated definite integral (see (6.17)) and the smallest root, $q_c = q_c(y, \bar{\lambda})$, of the equation (see Appendix)

$$2\cos q_c + y(\sin q_c)/q_c - 2\sqrt{\bar{\lambda}} = 0. \tag{6.2}$$

This equation determines the regions in which the scaled variables y and $\bar{\lambda}$ are important, depending on which part of the equation can be neglected in evaluating the leading term of q_c.

Once again we begin our analysis of the spherical constraint equation at (4.26). The methods of dealing with I_2 (see (5.2)) closely parallel those in the preceding section with the result expressed in (5.19). Thus, we proceed to analyse I_1 defined by (5.2). In the scaling regime $\lambda < n^{-1}$, the leading term of the critical value of z is given by (see Appendix)

$$z_c = -\lambda/n. \tag{6.3}$$

Hence, we consider complex z in the semi-annulus $\Omega = \Omega_1 \cup \Omega_2$ defined by

$$\begin{aligned} &\Omega \equiv \{z : \lambda < \sqrt{|z|} < (\lambda/n)^{1/2}, \operatorname{Im} z > 0\}, \\ &\Omega_1 = \Omega \cap \{z : \operatorname{Re} z \geq 0\}, \qquad \Omega_2 = \Omega \cap \{z : \operatorname{Re} z < 0\}. \end{aligned} \tag{6.4}$$

The basic strategy is to evaluate I_1 exactly (in principle) for $z \in \Omega_1$. Since I_1 is analytic in Ω, it can be continued into Ω_2, and an L^∞ version of the Paley–Weiner theorem (see Rudin 1974 p 264) can then be used to continue the function I_1 as a single-valued function onto the segment of the negative real line where $\lambda < \sqrt{|z|} < (\lambda/n)^{1/2}$, which is of primary interest.

In the region Ω_1, we use the fact that $\lambda < \sqrt{|z|}$ to write Y_λ^{-1} in the form of the expansion

$$\frac{1}{Y_\lambda} = \frac{1}{(2-\lambda)(p^2-1)^{1/2}} \sum_{j=0}^{\infty} (-1)^j u^j \tag{6.5}$$

where $u \equiv \lambda p[(2-\lambda)(p^2-1)^{1/2}]^{-1}$. This leads to the identity

$$I_1 = -\frac{(2\pi)^{-2}}{2} \frac{\lambda}{2-\lambda} \iint_0^{\pi} \mathrm{d}\theta\, \mathrm{d}\phi (p^2-1)^{-3/2} \sum_{j=0}^{\infty} (-1)^j u^j. \tag{6.6}$$

These integrals can be expanded in a series in powers of $\lambda z^{-1/2}$, in a way similar to the Watson functions. This will not be necessary, however, for our purposes. If we subtract off the term $(4\pi)^{-1} \ln[(p^2-1)^{1/2}/Y_\lambda]_{\theta=\phi=0}$, which we will show arises from I_2, then we eliminate the leading terms and establish the bound

$$I_1 - (4\lambda)^{-1} \ln[(p^2-1)^{1/2}/Y_\lambda]_{\theta=\phi=0} - (4\lambda)^{-1} \ln 2 = \mathrm{O}(\lambda n^{-1}) \qquad (\lambda \ll n^{-1}). \tag{6.7}$$

With the identity

$$\begin{aligned} -\ln[F + (F^2 - G^2)^{1/2}]_{\theta=\phi=0} \\ = n \ln Y_+|_{\theta=\phi=0} - \ln[(p^2-1)^{1/2}/Y_\lambda]_{\theta=\phi=0} - 2\ln[\sqrt{A_0} + (A_0 + 4\sqrt{\lambda})^{1/2}] \end{aligned} \tag{6.8}$$

we may write the spherical constraint equation in the form

$$\begin{aligned} 2K = W_3(0) + \frac{1}{2\pi n} \ln 2 + \frac{1}{4\pi n} \ln[1 + z/2 + (z + z^2/4)^{1/2}] \\ - \frac{1}{2\pi n} \ln[\sqrt{A_0} + (A_0 + 4\sqrt{\lambda})^{1/2}] + \mathrm{O}(\lambda n^{-1}). \end{aligned} \tag{6.9}$$

The shift in critical temperature can then be shown to have the form

$$K_c(\lambda = 0) - K_c(\lambda) = \mathrm{O}(\lambda n^{-1}) \tag{6.10}$$

in the scaling region $\lambda \ll n^{-1}$, or $y \to 0$.

We defer the discussion of equation (6.9) until § 7. At present we consider the scaling crossover between the two situations we have analysed, namely λ fixed and $\lambda < n^{-1}$.

We consider the integral I_1 first and show that an appropriate scaling function makes the transition from (5.10) for λ fixed, to (6.9) in which λ approaches zero faster than n^{-1}. To analyse I_1 in the general case, we write

$$\begin{aligned} I_1 = S_1 + S_2 + S_3 \\ \equiv \pi^{-2} \iint_0^{\pi} \frac{\lambda}{2Y_\lambda} \mathrm{d}\theta\, \mathrm{d}\phi + \pi^{-2} \iint_0^{\pi} \frac{-p}{2(p^2-1)} \mathrm{d}\theta\, \mathrm{d}\phi \\ + \pi^{-2} \iint_0^{\pi} \frac{(2-\lambda)p}{2(p^2-1)^{1/2} Y_\lambda} \mathrm{d}\theta\, \mathrm{d}\phi. \end{aligned} \tag{6.11}$$

The region of integration can be decomposed into R and R' where

$$R \equiv \{(\theta, \phi);\ \theta > 0,\ \phi > 0;\ \theta^2 + \phi^2 < \pi\}$$
$$R' \equiv \{(\theta, \phi):\ 0 \leq \theta,\ \phi \leq \pi\}\backslash R. \tag{6.12}$$

In each of the integrals in (6.11), the portion of the integral in R' may be replaced with the corresponding integrand in which the z has been replaced by zero without a change of more than $O(|z|^{1/2})$. In the region R, we consider the differences

$$D_i \equiv \iint_R \{[F_i(z) - \tilde{F}_i(z)] - [F_i(0) - \tilde{F}_i(0)]\}\, d\theta\, d\phi, \qquad i = 1, 2, 3, \tag{6.13}$$

where $F_i(z)$ are the integrands in S_i, and $\tilde{F}_i(z)$ indicates that ω^2 has been replaced by r^2 in the function. By using the types of methods discussed in § 5 one may show that the differences D_i are $O(z)$. Hence, we may write

$$n^{-1}\pi^2 I_1 = n^{-1} \iint_R \frac{-\lambda}{2(\tilde{p}^2 - 1)\tilde{Y}_\lambda}\, d\theta\, d\phi + n^{-1} \iint_{R'} \left[\frac{-\lambda}{2(\tilde{p}^2 - 1)\tilde{Y}_\lambda}\right]_{z=0} d\theta\, d\phi$$
$$+ n^{-1} \iint_R \left[\frac{-\lambda}{2(p^2 - 1)Y_\lambda}\right]_{z=0} - \left[\frac{-\lambda}{2(\tilde{p}^2 - 1)\tilde{Y}_\lambda}\right]_{z=0} d\theta\, d\phi + O(xn^{-2}, n^{-2}), \tag{6.14}$$

in which only the first integral is a function of z. The last two integrals do not contribute in a significant way since they are simply of the form $n^{-1}g_1(\lambda)$ and $n^{-1}g_2(\lambda)$, for some functions g_1 and g_2 defined by (6.14). Thus, it is the first integral which we analyse in greater detail. Since z_c ranges between $-\pi^2/n^2$ and $-\lambda/n$ as the scaling regime changes from λ fixed to $\lambda \to 0$ faster than n^{-1}, it is convenient to write z as

$$z = -q^2/n^2 \tag{6.15}$$

so that q^2 is expressible in terms of the scaling variable x (see (5.6)) and critical solution q_c (see (A10)) as

$$q = -x + q_c^2. \tag{6.16}$$

Having defined these variables, we analyse the first integral by (i) changing to polar coordinates so that $r^2 \equiv \theta^2 + \phi^2$; the angular integration yields a multiplicative factor of $\pi/2$; (ii) rescaling the integration from r to nr; (iii) showing that the upper limit of πn may be extended to $+\infty$ without an error of more than n^{-2}; and finally (iv) allowing z to approach the negative real line from the upper half of the complex plane (in effect adding $i\epsilon$ to z and then taking the limit as $\epsilon \to 0$ after the integral) which we denote by placing a bar through the integral sign. Thus, the first and principal part of $n^{-1}\pi^2 I_1$ may be expressed as

$$n^{-1}\pi^2 I_{1p} \equiv n^{-1}\frac{\pi}{2} \int_0^\infty \frac{-yr\, dr}{2[(-q_c^2 + x + r^2) + [(1-\bar{\lambda})^2/4y^2](-q_c^2 + x + r^2)^2]}$$
$$\times \left[y\left(1 + \frac{(1-\bar{\lambda})^2}{2y^2}(-q_c^2 + x + r^2)\right) + (2 - \lambda)\right.$$
$$\left.\times \left((-q_c^2 + x + r^2)\frac{(1-\bar{\lambda})^2}{4y^2}(-q_c^2 + x + r^2)^2\right)^{1/2}\right]^{-1}$$
$$+ O(xn^{-2}, n^{-2}) \tag{6.17}$$

where $y = n\lambda$ is the scaling variable previously defined.

We may now write the spherical constraint equation as

$$2K = W_3(z)+n^{-1}I_{1p}(x, y, q_c, \bar{\lambda})+n^{-1}g_1(\lambda)+n^{-1}g_2(\lambda)$$
$$+(4\pi n)^{-1}\{\ln 2+n\ln Y_+-\ln[(p^2-1)^{1/2}/Y_\lambda]_{\theta=\phi=0}$$
$$-2\ln[\sqrt{A_0}+(A_0+4\sqrt{\bar{\lambda}})^{1/2}]\}+O(xn^{-2}, n^{-2}) \qquad (6.18)$$

which may be simplified further to

$$2K = W_3(0)+n^{-1}I_{1p}(x, y, q_c, \bar{\lambda})-(4\pi n)^{-1}\ln\left[\frac{(x-q_c^2)^{1/2}}{y+(2-\lambda)(x-q_c^2)^{1/2}}\right]$$
$$+n^{-1}g_1(\lambda)+n^{-1}g_2(\lambda)+(4\pi n)^{-1}\ln 2$$
$$-(2\pi n)^{-1}\ln[\sqrt{A_0}+(A_0+4\sqrt{\bar{\lambda}})^{1/2}]+O(xn^{-2}, n^{-2}). \qquad (6.19)$$

It is appropriate at this stage to put the term

$$H(\lambda, n, z, z_c)\equiv\ln(\sqrt{A_0}+A_0+4\sqrt{\bar{\lambda}}) \qquad (6.20)$$

into a form in which the crossover behaviour is more transparent. In particular it is desirable to write the function in a form involving the scaled variables of both regimes. As shown in the Appendix, the function A_0 can be written, to sufficiently high order in n^{-1} for our purposes, as

$$A_0\cong 2\cosh n\sqrt{z}+n\frac{\sinh n\sqrt{z}}{n\sqrt{z}}-2\sqrt{\bar{\lambda}}. \qquad (6.21)$$

In terms of the scaling variables x and y, and the implicit function $q_c=q_c(y, \bar{\lambda})$ given by the largest root of (6.2), A_0 can be written

$$A_0\cong 2\cosh[x-q_c^2(y, \bar{\lambda})]^{1/2}+y\frac{\sinh[x-q_c^2(y, \bar{\lambda})]^{1/2}}{[x-q_c^2(y, \bar{\lambda})]^{1/2}}-2\sqrt{\bar{\lambda}}. \qquad (6.22)$$

Defining $H_\pm(x, y, \bar{\lambda})$ by

$$H_\pm(x, y, \bar{\lambda})=2\cosh[x-q_c^2(y, \bar{\lambda})]^{1/2}+y\frac{\sinh[x-q_c^2(y, \bar{\lambda})]^{1/2}}{[x-q_c^2(y, \bar{\lambda})]^{1/2}}\pm 2\sqrt{\bar{\lambda}} \qquad (6.23)$$

we may write $H(\lambda, n, z, z_c)$ in terms of both sets of scaled variables as

$$H=H(x, y, \bar{\lambda})=\ln[(H_+(x, y, \bar{\lambda}))^{1/2}+(H_-(x, y, \bar{\lambda}))^{1/2}]+O(xn^{-2}, n^{-2}). \qquad (6.24)$$

The final form of the spherical constraint equation is then

$$2K = W_3(0)+n^{-1}I_{1p}(x, y, q_c, \bar{\lambda})-(4\pi n)^{-1}\ln\left[\frac{(x-q_c^2)^{1/2}}{y+(1+\bar{\lambda})(x-q_c^2)^{1/2}}\right]$$
$$+n^{-1}[g_1(\lambda)+g_2(\lambda)]+(4\pi n)^{-1}\ln 2-(2\pi n)^{-1}H(x, y, \bar{\lambda})+O(xn^{-2}, n^{-2}), \qquad (6.25)$$

where to recapitulate, I_{1p} is defined in (6.17), $g_1(\lambda)$ and $g_2(\lambda)$ are given by (6.14) while $H(x, y, \bar{\lambda})$ is given by (6.24).

The above expression for the spherical constraint reduces to the expressions (5.21) or (6.9), respectively, as one specialises to $y\gg 1$ (λ fixed, non-zero) or $\bar{\lambda}\sim 1$.

The most important part of the crossover behaviour occurs within the term $H(x, y, \bar{\lambda})$. We know *a priori* that the spherical constraint equation must display drastically different behaviour in the two scaling regimes. The role of all but the last terms in (6.25) is essentially to provide the appropriate constants and to vanish as $\lambda \to 0$. The function $H(x, y, \bar{\lambda})$ is chiefly responsible for the major changes necessary in the spherical constraint equation such as divergence at $\lambda = 1$, creation of a $\phi^{1/2}$ term at $\lambda = 0$, etc. A discussion of the origins of these transitions will be the subject of the next section.

7. General scaling behaviour and thermodynamic functions

In the first part of this section we discuss the qualitative scaling aspects of the spherical constraint equation in the form (6.25) which has, as its limiting forms, equations (5.21) and (6.9) for the λ fixed, non-zero and $\lambda \to 0$ faster than n^{-1} scaling regimes. In the latter part of this section we discuss the implications for various thermodynamic functions. The functions responsible for the crossover behaviour must (i) restore the term $-z^{1/2}/4\pi = -\phi^{1/2}/4\pi$ for the pure system ($\lambda = 0$); (ii) create a logarithmic term, $\ln \phi$, for the decoupled system ($\lambda = 1$); (iii) create a term of the form $\phi^{1/2}$ with a large coefficient (which turns out to be $O(n^{1/2})$) for the intermediate situation of arbitrary, fixed λ $(0 < \lambda < 1)$ which 'hooks up' the spherical constraint functions of the situations (i) and (ii) (see figure 3).

We begin by studying the scaling regime in which λ does not approach zero, i.e. λ is fixed or $\lambda \to 1$, which is governed by equation (5.21). At the limit $\lambda \to 1$ the planes of impurities decouple the system so that one has the finite size effect studied by Barber and Fisher. To see that this is in fact the case, one may write (5.21) as

$$2K = W_3(0) + \frac{1}{n}\left(W_3(0) - \tfrac{1}{2}W_2(4) - \frac{7}{8\pi}\ln 2\right) - \frac{1}{n}\frac{1}{4\pi}\ln A_0 + O(xn^{-2}, n^{-2}). \tag{7.1}$$

Upon writing the identity

$$\begin{aligned} A_0 &= Y_+^n + Y_-^n + \tfrac{1}{2}(p^2-1)^{-1/2}(Y_+^{n-1} - Y_-^{n-1}) \\ &= \frac{Y_+^{n+1} - Y_-^{n+1}}{2(p^2-1)^{1/2}}, \end{aligned} \tag{7.2}$$

which is approximated to the order of interest by

$$\frac{A_0}{n} = \frac{\sin[(n+1)|z|^{1/2}]}{n|z|^{1/2}} \qquad (z<0), \tag{7.3}$$

one has the result, identical to that of Barber and Fisher (1973), that

$$\begin{aligned} 2K &= W_3(0) + (W_3(0) - \tfrac{1}{2}W_2(4) - 7\ln 2/8\pi)/n \\ &\quad - (\ln n)/4\pi n - R_{1,0}[(x/\pi^2) - 1]/4\pi n + O(xn^{-2}, n^{-2}) \end{aligned} \tag{7.4}$$

where $R_{1,0}(x) = \ln[\sinh(\pi x^{1/2})/\pi x^{1/2}]$ is the remnant function defined in Barber and Fisher (1973), Fisher and Barber (1972) by

$$R_{1,0}(x) = \sum_{r=1}^{\infty} \ln(1 + x/r^2). \tag{7.5}$$

As the critical point is approached (i.e. $x \to 0$ in terms of the scaled variables) the expected logarithmic divergence arises from the remnant function since

$$R_{1,0}(x) \sim \ln(1+x), \qquad x \to -1+. \tag{7.6}$$

Hence, the origin of the logarithmic divergence is in the term $\ln[\sqrt{A_0}+(A_0+4\sqrt{\bar{\lambda}})^{1/2}]$. For $\bar{\lambda} \neq 1$ (i.e. $\lambda \neq 0$), this divergence is prevented by means of the $4\sqrt{\bar{\lambda}}$ term within the radical. As noted earlier, $\bar{\lambda}$ itself is a scaling variable in this regime which is mainly responsible for the transition from an essentially two-dimensional system to one which is three-dimensional with impurities.

To examine the behaviour at the opposing end, near $\lambda = 0$, one may begin by writing A_0 as $A_0 \cong (z-z_c)(\partial A/\partial z)_{z=z_c}$. Performing the differentiation and substituting $z_c = -\lambda/n$ (see the Appendix), one has to leading order $A_0 \cong \phi n^2$, so that

$$(2\pi n)^{-1} \ln[(A_0+A_0+4\bar{\lambda})^{1/2}] \cong (2\pi n)^{-1} \ln[n\phi^{1/2}+(n^2\phi+4)^{1/2}]. \tag{7.7}$$

As $x = n^2\phi \to 0$, this term becomes $\phi^{1/2}/4\pi n$ plus a constant term $(\ln 2)/2\pi n$ (which cancels with a previous such constant) and one recovers the pure 3D behaviour

$$2K \cong W_3(0) - z^{1/2}/4\pi. \tag{7.8}$$

Using the same type of approximations we find $A_0 \approx \phi n^3/2\pi^2$ for λ fixed, so that the leading term is $n^{1/2}\phi^{1/2}$ (for a very small range of ϕ, namely $\phi < n^{-3}$). Thus, the situation is as illustrated in figure 3: for intermediate λ, one has a $\phi^{1/2}$ term characteristic of a three-dimensional system; however, it has a large (negative) slope. As λ approaches zero the coefficient of $\phi^{1/2}$ diminishes (in absolute value), i.e. the slope becomes smaller, while z_c approaches the pure value, and the spherical constraint curve 'hooks up' with the pure system. Alternatively as λ approaches unity (for fixed n) the slope becomes larger until the $\phi^{1/2}$ term eventually becomes logarithmic, thereby connecting with the logarithmic divergence of a two-dimensional system.

As noted in § 6, $\ln[\sqrt{A_0}+(A_0+4\sqrt{\bar{\lambda}})^{1/2}]$ can be written in the form of $H(x, y, \bar{\lambda})$ defined by (6.24). The various limits discussed above can also be seen directly from this form. In particular, at $\bar{\lambda} = 0$, $H_- = H_+$, leading to the logarithmic divergence at T_c from the $\ln A_0$ term. The behaviour of the spherical constraint for intermediate values of λ and n is governed by the rather complicated expression for $H(x, y, \bar{\lambda})$ which takes on a much simpler form, as discussed above, when the extremes $\lambda = 0$ or $\lambda = 1$ are approached.

The scaling behaviour of the spherical constraint function $\Sigma_q (s-\mu_q)^{-1}$ determines the scaling behaviour of various thermodynamic functions such as the specific heat, the entropy and the internal energy. In particular, the spherical constraint equation we have obtained yields the spherical field s as a function of T; hence the zero-field specific heat per spin, which is given by (2.15) as

$$C_H(T) = \tfrac{1}{2}k_B - (\partial s/\partial T)_{h=0,S}, \tag{7.9}$$

can be evaluated explicitly. The scaling and crossover behaviour discussed for the spherical constraint equation thus applies also to the specific heat. In particular, in the region of fixed and non-zero λ one has a spherical constraint of the form

$$2K \approx W_3(z) + n^{-1} f(\bar{\lambda}, x) \tag{7.10}$$

where $f(\bar{\lambda}, x)$ is defined explicitly by (5.21), so that

$$\left(\frac{\partial \phi}{\partial T}\right)_{h=0,S} \approx \frac{-2J/k_B T^2}{[W_3'(z) + n^{-1}\, \partial f(\bar{\lambda}, x)/\partial \phi]_S} \tag{7.11}$$

and the specific heat is given by

$$C_H(T) \approx C_H(\lambda = 0, T) + n^{-1} 2J^2/k_B T^2 [2f(\bar{\lambda}, x)/\partial\phi]_S, \tag{7.12}$$

where the value of ϕ, or equivalently x, is determined by (7.10). Analogous remarks apply to the other λ regions. In a similar way the entropy may be evaluated, using (2.14) and then integrating the spherical constraint function $\Sigma_q (s-\mu_q)^{-1}$ over s. Various other thermodynamic variables such as the internal energy may be obtained from these thermodynamic functions.

We note, however, that the susceptibility cannot be calculated from the spherical constraint equation directly. The zero-field susceptibility is given by

$$\chi_0(T) = \frac{1}{2N} \sum_{q=0}^{N-1} \frac{|\epsilon_q|^2}{s-\mu_q}, \tag{7.13}$$

where the variables ϵ_q are defined by (2.10) as sums of column elements of the diagonalising matrix $\boldsymbol{U}$. For the pure system, $\epsilon_q = N^{-1/2}\delta_{q,0}$, so that $\chi_0(T)$ takes on a particularly simple form. In the more general case of impurities, however, the ϵ_q will not be easily expressible in closed form and further analysis is necessary to find the asymptotic behaviour of the eigenvectors. This seems to be an intrinsic difficulty since other ways of computing the susceptibility eventually entail further information on eigenvalues and eigenvectors.

8. The spherical model with impurities in other dimensions and co-dimensions

In the preceding sections the problem of two-dimensional impurities in a three-dimensional lattice was discussed in detail. It is of interest to consider the problem of regular impurities in the spherical model in other dimensions and co-dimensions (i.e., the dimensionality of the space minus the dimensionality of the impurities). In this section we formulate the problem in various other cases, although the detailed analysis is not carried out.

The problem which is closest to the one we have analysed is that which has co-dimension equal to one for an arbitrary space dimensionality. For integer dimensions, d, the analysis of $\det(s\boldsymbol{I}-\boldsymbol{J})$ closely parallels the $d=3$ case. The main difference, of course, is that the product over three indices becomes a product over d indices, which is eventually transformed into a d-fold integral. Explicitly, for $d=4$, one has an expression (compare with (3.17))

$$J^n \det(s\boldsymbol{I}-\boldsymbol{J}) = \prod_{j,k,l,q} [Y_+^n + Y_-^n - \lambda(Y_+^{n-1} - Y_-^{n-1})/X - 2\sqrt{\lambda}\cos\gamma_l] \tag{8.1}$$

in which X, $Y_\pm$ are redefined by modifying the variable a in expression (3.12) to

$$a = s/J - 2\alpha_j - 2\beta_k - 2\omega_q, \tag{8.2}$$

where $\omega_q \equiv \cos(2\pi q/N_4)$ and N_4 is the length of the lattice in the fourth direction, so that $N = N_1N_2N_3N_4n$. The algebraic identities of § 4 are all valid with the new definitions of X and $Y_\pm$. For three dimensions the behaviour of the pure system was recovered through the identity

$$W_3(z) = (2\pi)^{-2} \iint_0^{2\pi} \mathrm{d}\theta\, \mathrm{d}\phi\, \tfrac{1}{2}(p^2-1)^{-1/2}. \tag{8.3}$$

A very similar situation occurs for four dimensions where

$$W_4(z) = (2\pi)^{-3} \iiint^{2\pi} \mathrm{d}\theta\, \mathrm{d}\phi\, \mathrm{d}\omega\, \tfrac{1}{2}(p^2-1)^{-1/2}, \tag{8.4}$$

and $(p^2-1)^{1/2} = \frac{1}{2}X$ is defined in the four-dimensional sense as discussed above. For the system *with* impurities an analysis similar to $d = 3$ may be carried out beginning with (4.26) upon appropriate modification of X, $Y_{\pm}$, Y_{α} via (8.2) and addition of a third integral, $\int_0^{2\pi} \mathrm{d}\omega$.

For non-integral dimensions, d, one must essentially define what is meant by the d-dimensional integrals in (4.26). A basic method (M E Fisher, unpublished) for generalising a d-dimensional integral to a non-integer d is by using the identities (Montroll 1955, Maradudin *et al* 1960)

$$t^{-1} = \int_0^{\infty} \mathrm{e}^{-tx}\, \mathrm{d}x, \qquad \mathrm{I}_0(t) = (2\pi)^{-1} \int_0^{2\pi} \mathrm{e}^{t\cos\theta}\, \mathrm{d}\theta, \tag{8.5}$$

where $\mathrm{I}_0(t)$ is the Bessel function of zero order and pure imaginary argument. For example, functions $W_d(\phi)$ defined by (2.19) may be written

$$W_d(\phi) = \tfrac{1}{2} \int_0^{\infty} \mathrm{e}^{-\phi t/2} [\mathrm{e}^{-t} \mathrm{I}_0(t)]^d\, \mathrm{d}t. \tag{8.6}$$

The dimensionality is thus explicit in (8.6), so that this expression defines the functions for non-integral d.

Impurity problems with co-dimension two include the work of Au-Yang *et al* (1976; Au-Yang 1976, Fisher and Au-Yang 1975) in which they considered regularly spaced point impurities in a two-dimensional Ising model. Since the spherical model in two-dimensional space does not exhibit a phase transition, one must consider $d \geqslant 3$. For $d = 3$ the problem becomes that of line impurities of separation distance m and n, respectively in the two directions. The determinant of $s\boldsymbol{I} - \boldsymbol{J}$ is evaluated in a way similar to that employed in § 3, i.e. by repeatedly using cyclic transformations to reduce the original matrix to one which is a manageable $n \times n$. However, the following trick must be employed to ensure that the transformed matrix is one whose determinant can be obtained in closed form. If we use the notation $B(i, j)_{k,l}$ to denote the (i, j) element of the (k, l) block of the block matrix B, and define the block matrix C by

$$[C(i, j)]_{k,l} = [B(k, l)]_{i,j} \tag{8.7}$$

then one has the equality $\det B = \det C$. For impurities placed on the bonds which lie perpendicular to the lines the final result may be expressed in the form:

$$\ln \det(s\boldsymbol{I} - \boldsymbol{J}) = \ln \det(s\boldsymbol{I} - \boldsymbol{J}_0) + \sum \ln\{1 + (J - J')[C_0^{-1}(m, m)]_{n,n}\} \tag{8.8}$$

where the sum is over $j = 1, \ldots, N_3$, $k = 1, \ldots, N_2$, $l = 1, \ldots, N_1$; $\alpha_j = 2\pi j/N_3$, $\theta_k \equiv 2\pi k/N_2$, $\beta_l = 2\pi l/N_l$, J_0 is the matrix of pure interactions, and

$$[C_0^{-1}(m, m)]_{n,n} = (mn)^{-1} \sum_{u=1}^{m} \sum_{v=1}^{n} [s - 2\alpha_j J - 2J \cos(2\pi u - \beta_l)/m$$
$$- 2J \cos(2\pi v - \theta_k)/n]^{-1}. \tag{8.9}$$

In the thermodynamic limit ($N_1, N_2, N_3 \to \infty$), the sums over j, k and l become integrals over angle variables from 0 to 2π, multiplied by $(2\pi)^{-1}$. Thus, the spherical constraint equation and the critical temperature, $T_c(m, n)$, can be obtained as an expansion in powers of $(mn)^{-1}$ upon (i) analysing the sum (8.9), and (ii) evaluating the largest eigenvalue of $(s\boldsymbol{I}-\boldsymbol{J})$. An analysis of $[C_0^{-1}(m, m)]_{n,n}$ for asymptotically large m, n is carried out in Au-Yang *et al* (1976), while the largest eigenvalue of $s\boldsymbol{I}-\boldsymbol{J}$ is presumably obtainable by the same method as that which is employed in the Appendix. The critical value of the spherical field, s_c, can also be determined by a method similar to that used by Au-Yang *et al* (1976) to determine the critical temperature for the two-dimensional Ising model with point impurities. The basic idea is that the only source for a singularity in (8.8) is the vanishing of the argument of the logarithms. The second logarithm in (8.8) must be responsible for (i) creating a singularity at the new critical point and (ii) cancelling the singularity of the first logarithm, i.e. the critical point of the pure system. Hence, the critical value of the spherical field is determined by the appropriate solution to

$$(J'-J)[C_0^{-1}(m, m)]_{n,n}=1. \tag{8.10}$$

It is easy to verify that such a singularity does indeed lead to the $(s-s_c)^{1/2}$ behaviour upon triple integration.

Finally, we comment on the analysis of point impurities in the spherical model. For a concentration x of regular spaced point impurities, the free energy may be expected to assume the form (see Fisher and Au-Yang (1975))

$$f(T, x)\cong A(x)[T-T_c(x)]^{2-\alpha}. \tag{8.11}$$

This is just the assumption that the critical exponents do not vary with impurities. For small concentrations, x, one may write

$$\begin{aligned} f(T, x)&=f_0(T, x)+xf_1(T)+\ldots \\ f_1(T)&=\left[\frac{\partial f(T, x)}{\partial x}\right]_{x=0}, \end{aligned} \tag{8.12}$$

so that the expansion of the right-hand side of (8.11) implies

$$f_1(T)=A_1[T-T_c(0)]+(2-\alpha)A_0\left[\frac{\partial T_c(x)}{\partial x}\right]_{x=0}[T-T_c(0)]^{-\alpha+1} \tag{8.13}$$

where $A_0\equiv A(0)$, $A_1\equiv[\partial A(x)/\partial x]_{x=0}$. The function $f_1(t)$ is the incremental free energy per impurity. Since A_0 is known from the pure spherical model, one may obtain $A_1=[\partial A(x)/\partial x]_{x=0}$, i.e. a measure of the change in amplitude, by determining the critical shift $T_c(x)$ and the incremental free energy. The incremental free energy $f_1(T)$ may be analysed using information about the expectation values of the pure system in the following way.

Let $\mathcal{H}_0$ be the Hamiltonian for the pure system and $\mathcal{H}_1$ the Hamiltonian for the system with a single bond impurity so that $\mathcal{H}_1-\mathcal{H}_0=K'\sigma_0\sigma_1$. Then

$$\mathrm{e}^{f_1(T)}=\exp[F(\mathcal{H}_1)-F(\mathcal{H}_0)]=\langle\exp(K'\sigma_0\sigma_1)\rangle=\sum_{j=1}^{\infty}\frac{K'^j}{j!}\langle\sigma_0^j\sigma_1^j\rangle. \tag{8.14}$$

The expectation values $\sigma_0^j\sigma_1^j$ may of course be computed as derivatives of the free energy, i.e.

$$\langle\sigma_0\sigma_1\rangle=\partial F/\partial J_{01}, \qquad \langle\sigma_0^2\sigma_1^2\rangle=(\partial F/\partial J_{01})^2+\partial^2F/\partial J_{01}^2, \tag{8.15}$$

etc.

This concludes our comments on impurities in the spherical model in various dimensions and co-dimensions.

Appendix: the largest eigenvalue of $sI - J$

In this Appendix we examine the function $A(\theta, \phi, \psi)$ (see equation (4.2)) at $\theta = \phi = \psi = 0$ and analyse its leading zero as a function of $z = s/J - 6$. It is evident from the spherical constraint equation (4.1) that the largest zero is the critical value of z, denoted by z_c. We write the identities (for n even)

$$Y_+^n + Y_-^n = 2\cosh[n \ln(p + (p^2-1)^{1/2})] \tag{A1}$$

$$Y_+^{n-1} - Y_-^{n-1} = 2\sinh\{n \ln[p + (p^2-1)^{1/2}]\}, \tag{A2}$$

and note that for $\theta = \phi = \psi = 0$, $p = 1 + z/2$ and $(p^2-1)^{1/2} = (z + z^2/4)^{1/2}$. Thus (4.2) can be written as the identity $[A_0 \equiv A(0, 0, 0)]$

$$A_0 = 2\cosh\{n \ln[1 + z/2 + (z + z^2/4)^{1/2}]\} + \frac{\lambda \sinh[n \ln(1 + z/2 + (z+z^2/4)^{1/2})]}{(z + z^2/4)^{1/2}} - 2\sqrt{\lambda}. \tag{A3}$$

From this one can conclude $0 \geqslant z_c > -1/n$ and that the leading coefficient in the expansion of z_c can be obtained from the simplified expression

$$A_0 \cong 2\cosh n\sqrt{z} + n\lambda \frac{\sinh n\sqrt{z}}{n\sqrt{z}} - 2\sqrt{\lambda}$$

$$= 2\cos n\sqrt{|z|} + n\lambda \frac{\sin n\sqrt{|z|}}{n\sqrt{|z|}} - 2\sqrt{\lambda} \qquad \text{(for } z < 0\text{).} \tag{A4}$$

For a pure system ($\lambda = 0$), the largest solution is $z = 0$. In the case of fixed non-zero λ, so that λ is eventually large in comparison with n^{-1}, one can let z assume the form

$$n|z|^{1/2} = a + b/n \tag{A5}$$

and asymptotically determine the coefficients a and b from (A4) by utilising the double-angle formulae for sine and cosine. This yields the result

$$|z_c|^{1/2} = \pi n^{-1} + [-2\pi(1+\sqrt{\lambda})/\lambda + \pi]n^{-2} + O(n^{-3}) \tag{A6}$$

which in the special case of separating planes ($\lambda = 1$) is just

$$|z_c|^{1/2} = \pi/(n+1) + O(n^{-3}). \tag{A7}$$

Alternatively, in a scaling limit in which $\lambda \ll 1/n$, one can use a similar analysis to obtain

$$|z_c|^{1/2} = (\lambda/n)^{1/2} + O(n^{-2}). \tag{A8}$$

For λ in an arbitrary scaling regime, we express z_c in the form

$$z_c = -q_c^2/n^2 + (\text{higher order in } n^{-1}) \tag{A9}$$

where $q_c = q_c(y, \bar{\lambda})$ is the solution to

$$2\cos q_c + y\frac{\sin q_c}{q_c} - 2\sqrt{\bar{\lambda}} = 0 \tag{A10}$$

and $y \equiv n\lambda$.

The variable q_c is O(1), since $q_c^2 \leqslant \pi$; consequently $z_c = O(n^{-2})$ in all scaling regimes.

We note also that, as a function of the complex variable z, the function appearing on the right-hand side of (4.1) is analytic in the complex z plane outside a cut of finite length along the negative real axis from $-z_c$ to approximately $-4d$.

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