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Critical temperature of finite systems in d dimensions

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Abstract. The critical temperature of an Ising system consisting of n ($d-1$) dimensional layers in d dimensions is estimated for large n from the properties of random and self-avoiding walks (SAW) in the finite system. Denoting the deviation of $T_c(n)$ from $T_c(\infty)$ by $1/n^\lambda$ it is found that there are two contributions, a finite size effect which applies both to a torus and a strip and for which $\lambda = d-2+\eta$, and a free boundary effect which applies to a strip alone and for which $\lambda = 1/\nu_d$. (ν_d, η are exponents associated with the spin pair correlation function using the standard notation of Fisher.) The results are based on a perturbation expansion for SAW which should be reliable for $d \geq 4$, but which needs further examination when $d = 3$. Some, but not all, of the above features are in agreement with the results of Fisher and Barber for the spherical model.

1. Introduction

A number of theoretical calculations in recent years have been devoted to the effect of the finite size of a system on its critical behaviour. Earlier work had been concerned with critical surface exponents and rounding to a finite maximum (for a review of these aspects see Watson 1972). More recently attention has been focused on the transition from ($d-1$) dimensional critical behaviour to d dimensional critical behaviour in finite layers.

Allan (1970) investigated the transition in critical temperature from a two dimensional to a three dimensional Ising model by means of high temperature series expansions for the magnetic susceptibility. Calculations were undertaken for n plane square lattice layers with $n = 2, 3, 4$ and 5 using (a) free-surface boundary conditions, (b) periodic boundary conditions; an attempt was then made using the accurately known three dimensional value for $n = \infty$ to estimate the form of approach for large n . Writing

$$\epsilon(n) = \frac{T_c(\infty) - T_c(n)}{T_c(\infty)} \sim \frac{b}{n^\lambda}, \quad (1)$$

Allan suggested that his calculations were consistent with $\lambda = 1$ in case (a) and $1.56 \simeq 1/\nu_3$ in case (b), the first result being in accord with a naive mean field theory argument given by Fisher and Ferdinand (1967). However, Allan pointed out that as n increased the susceptibility series were too short for an accurate estimation of $T_c(n)$ since there was a crossover from three to two dimensional behaviour; hence the conclusions from such a double extrapolation process must be regarded as very tentative. More recently Fisher (1971) reported on more extensive calculations and suggested instead that $\lambda \simeq 1.56 \simeq 1/\nu_3$ in case (a) and $\lambda \simeq 2$ in case (b).

For the spherical model ($d \geq 3$) exact calculations by Fisher and Barber (1972) of the transition from a $(d-1)$ to d dimensional manifold show that $\lambda = 1$ in case (a) and $(d-2)$ in case (b). It is usually assumed (eg Wilson and Fisher 1972) that for $d \geq 4$ the exponents attain their mean field values independently of the model, hence the above results for the spherical model might be expected to apply to the Ising and Heisenberg models for $d \geq 4$. However, the above may be true only for bulk properties, and it is therefore worth looking around for any other information which might be available for the Ising and Heisenberg models.

It is the aim of the present paper to discuss the problem from the point of view of the general structure of high temperature series expansions for these models and to use the analogy between self-avoiding walks and the Ising model. We shall start with a brief introduction based on a recent publication (Domb 1972). The susceptibility, specific heat, and pair correlation function for the Ising model can be expanded at high temperatures in the form

$$x^{(\alpha)} = \sum c_N^{(\alpha)} w^N, \quad (w = \tanh \beta J) \quad (2)$$

where J is the interaction energy of a pair of parallel spins. The coefficients $c_N^{(\alpha)}$ are sums of connected graphs of certain types which can be constructed from bonds of the lattice weighted in a particular manner; we call these *Ising configurations*. The most important contribution to an Ising configuration is a self-avoiding walk (SAW) between two points of the lattice. We refer to the set of all Ising configurations connecting pairs of points on the lattice as an *Ising walk* (Brout 1972). In the publication mentioned above it is argued that an Ising walk is a SAW with a special type of repulsive interaction.

If we take only the SAW contribution to the coefficients into account we obtain the SAW approximation to the solution. The geometrical properties of SAW are not known exactly but reliable conjectures have been made as a result of extrapolation from exact enumerations and Monte Carlo runs (see eg Domb 1969). If we make a further approximation and ignore the self-avoiding condition on the walk we obtain the *random walk approximation*. Such an approximation should give correct results for sufficiently high d . It yields the Ornstein–Zernike expression for the pair correlation function (Domb 1968) and mean field values for the critical exponents.

In the present paper we shall confine our attention to the SAW approximation which we shall apply to n $(d-1)$ layers in d dimensions in a simple cubic type of structure with (i) free-surface boundary conditions, (ii) periodic boundary conditions. We can formulate the problem as follows. Consider all SAW of N steps starting from an origin in d dimensional space. Draw two $(d-1)$ dimensional hyperplane boundaries n layers apart containing the origin. For boundary conditions (i) any walk which once crosses the boundary is eliminated (but we must average over all possible positions of the origin among the n layers). For boundary conditions (ii) any walk which as a result of looping the torus $1, 2, \dots, r, \dots$ times becomes self-intersecting must be eliminated. The critical temperature of the $(d-1)$ layer system is determined by the number of surviving walks.

It is clear from the above description that more walks will be lost by (i) than by (ii) and hence the depression of critical temperature will be larger in the former case. We shall start with the random walk approximation and will apply a perturbation treatment to take account of the self-avoidance. This should lead to valid results when $d \geq 4$. When $d = 3$ we will try to draw some general conclusions based on the known behaviour of SAW.

2. Random walk approximation

There are two alternative methods of dealing with the properties of random walks in a finite strip.

- (i) The use of images (see eg Chandrasekhar 1943).
- (ii) The method of eigenvalues (Rubin 1972).

The first method takes account of the barrier by means of a suitably located image point. One can think of the barrier as causing a 'reflection' with an appropriate phase change, and for a finite strip successive reflections give rise to an infinite series of images. The second method, which has been used very effectively to deal with problems arising in the adsorption of a polymer chain at a free surface, constructs a series of difference equations relating the behaviour at layer t with that at layers $(t-1)$ and $(t+1)$. The matrix of these equations is found to be identical with that arising in the lattice dynamics of a linear chain, and hence the eigenvalues and eigenvectors can readily be calculated.

We shall use method (ii) to obtain exact expressions for the total number of walks of N steps, and the number at their starting point after N steps. However, we shall then find it convenient to revert to the physical picture of method (i) to give a geometrical interpretation of the result obtained.

Let $c_N(t)$ be the total number of walks which are at layer t after N steps. Then if $1 < t < n$ we have the relations

$$c_{N+1}(t) = (2d-2)c_N(t) + c_N(t-1) + c_N(t+1). \quad (3)$$

Equation (3) can be extended to $t = 1$ and $t = n$ provided we take

$$c_N(0) = c_N(n+1) = 0.$$

We write (3) in the form

$$\mathbf{c}_{N+1} = \mathbf{A}\mathbf{c}_N \quad (4)$$

where the matrix \mathbf{A} is identical with that which arises in the problem of a linear chain of harmonic oscillators with fixed ends.

The eigenvalue equations can be put in the form

$$\lambda x(r) = (2d-2)x(r) + x(r-1) + x(r+1). \quad (5)$$

Putting

$$x(r) = A \exp ir\theta + B \exp -ir\theta \quad (6)$$

we obtain

$$\lambda = (2d-2) + 2 \cos \theta = 2d - 4 \sin^2 \frac{1}{2}\theta. \quad (7)$$

To satisfy the boundary conditions at $t = 0$ and n we must have

$$\begin{aligned} B &= -A \\ \sin(n+1)\theta &= 0. \end{aligned} \quad (8)$$

Hence we find for the eigenvalues

$$\lambda_s = 2d - 4 \sin^2 \frac{s\pi}{2(n+1)} \quad (s = 1, 2, 3, \dots, n) \quad (9)$$

and for the eigenvectors

$$x_s(r) = \sin \frac{rs\pi}{n+1}. \tag{10}$$

To normalize the eigenvectors we must multiply by a factor $(x_s(1)^2 + \dots + x_s(n)^2)^{-1/2}$ which is easily shown to be $\{\frac{1}{2}(n+1)\}^{-1/2}$.

It is a straightforward matter to calculate the total number of walks of N steps which start from a particular t , by choosing an initial vector u_0 having 1 in the t th position and zero elsewhere, and expanding u_0 in terms of the eigenvectors x_s . If we then average from $t = 1$ to n we obtain the random walk approximation to the susceptibility coefficient in the form

$$c_N(\text{strip}) = \frac{2}{n(n+1)} \sum_{s=1,3,5,\dots} \cot^2 \frac{s\pi}{2(n+1)} \lambda_s^N. \tag{11}$$

To determine u_N the number of returns to the origin after N steps we must generate the space distribution of the $c_N(t)$. Define $c_N(t; l_1, \dots, l_{d-1})$ to be the number of walks at (l_1, \dots, l_{d-1}) in $(d-1)$ space after N steps. Write

$$Q_N(t; x_1, \dots, x_{d-1}) = \sum_{l_1, \dots, l_{d-1}} c_N(t; l_1, \dots, l_{d-1}) x_1^{l_1} \dots x_{d-1}^{l_{d-1}}. \tag{12}$$

Then it is easy to establish by analogy with (3) the relations

$$Q_{N+1}(t) = f Q_N(t) + Q_N(t-1) + Q_N(t+1) \tag{13}$$

where

$$f = x_1^{-1} + x_1 + x_2^{-1} + x_2 + \dots + x_{d-1}^{-1} + x_{d-1} \tag{14}$$

is the generating function for walks in $(d-1)$ space.

The matrix $\mathbf{A}(x_i)$ corresponding to (13) has exactly the same eigenvectors as \mathbf{A} in (4), but instead of (9) the eigenvalues are now

$$\lambda_s(f) = f + 2 - 4 \sin^2 \frac{s\pi}{2(n+1)} \quad (s = 1, 2, \dots, n). \tag{15}$$

For returns to the origin we must sort out the coefficient independent of x_i . By a similar procedure to that used before we find for the random walk approximation to the energy coefficient

$$u_N(\text{strip}) \simeq \frac{A_{d-1}}{nN^{(d-1)/2}} \sum_{s=1}^n \lambda_s^N. \tag{16}$$

Here A_{d-1} is the constant characterizing returns to the origin in $(d-1)$ dimensional space, that is, the number of such returns is $A_{d-1} \{2(d-1)\}^N / N^{(d-1)/2}$.

We can draw a number of conclusions from formulae (11) and (16). The critical temperature corresponds to the radius of convergence of the series (2) and is therefore given by

$$w_c^{-1} = \lim_{N \rightarrow \infty} |c_N|^{1/N} = \lambda_1 = 2d - 4 \sin^2 \frac{\pi}{2(n+1)}. \tag{17}$$

Hence we see on reference to (1) that for large d the correct value of λ is equal to 2, and we may reasonably term this the *true* mean field value. The *naive* mean field value of

$\lambda = 1$ quoted by Fisher and Ferdinand (1967) takes into account only the average change of coordination number, and not the adjustment of the mean field because of the presence of the boundary. This has already been pointed out by Binder and Hohenberg (1972), who give reference to earlier work which made use of ‘Ginzburg–Landau’ theory (see also Kaganov and Omel’yanchuk 1971).

Next we see that even for a modest value of n the eigenvalue spectrum is closely spaced, and it would be difficult to estimate the critical temperature accurately from extrapolation until relatively high values of N . The susceptibility series (11), in which the weighting of the second-largest eigenvalue is approximately $\frac{1}{9}$ of the largest eigenvalue, will yield a much better estimate than the specific heat series (16) in which the weightings are equal.

Although this approximation gives mean field exponents for all $d \geq 2$ there is a change of exponent in α_s , the singular part of the specific heat which changes from $2 - (d - 1)/2$ to $2 - d/2$. The manner in which this change is achieved will be clear on studying the behaviour of the coefficients in (16) for different values of N . When $N \gg n^2$ the largest eigenvalue dominates and the behaviour of the coefficients is $(d - 1)$ dimensional,

$$u_N \sim \frac{A_{d-1}}{nN^{(d-1)/2}} \lambda_1^N \tag{18}$$

However, when N decreases to become comparable with n^2 we have

$$c_N \sim \frac{A_{d-1}(2d)^N}{N^{d/2}} \sum_{s=1}^n \left(1 - \frac{s^2\pi^2}{n^2}\right)^{n^2} \sim \frac{A_{d-1}(2d)^N}{N^{d/2}} \sum_{s=1}^n \exp -s^2\pi^2 \sim \frac{A'(2d)^N}{N^{d/2}} \tag{19}$$

which is d dimensional behaviour. From this we can delineate the regions near T_c which correspond to $(d - 1)$ and d dimensional behaviour, and deduce that the rounding exponent (θ in Fisher and Barber’s notation) is equal to 2.

To calculate the critical surface exponents we must examine the behaviour of (11) and (16) for large n as far as the term in $1/n$. This requires careful treatment but we have been able to verify that both the susceptibility and specific heat satisfy the relation

$$\psi^x = \psi + \frac{1}{2} = \psi + \nu \tag{20}$$

where ψ^x represents the surface and ψ the bulk exponent.

For a torus the problem is simpler since there is no difference in behaviour for any starting point t . It is clear that the total number of walks, c_N , retains the d dimensional value of $(2d)^N$. However, the number of returns to the origin after N steps u_N , is changed, since it must now include walks which are at the origin as a result of looping the torus. Hence we may write

$$u_N(\text{torus}) = c_N(0, \mathbf{0}) + \sum_{s=1}^{\infty} (c_N(sn, \mathbf{0}) + c_N(-sn, \mathbf{0})) \tag{21}$$

where the first number p in $c_N(p, \mathbf{q})$ refers to the d th dimension, and the bold number \mathbf{q} refers to the remaining $(d - 1)$ dimensions. Using asymptotic expressions for the number of random walks in (21) (Domb 1970) we find that

$$u_N(\text{torus}) \simeq \frac{(2d)^N A_d}{N^{d/2}} \left(1 + 2 \sum_{s=1}^{\infty} \exp -\frac{ds^2 n^2}{2N}\right) \tag{22}$$

As in (16), if we examine (22) for different values of N we can delineate the regions of d dimensional behaviour ($N \ll n^2$) and $(d - 1)$ dimensional behaviour ($N \gg n^2$) and hence describe in detail the change of exponent.

We thus see that for a torus the random walk approximation leads to no change in critical temperature, and we must proceed to a higher approximation to find the order of magnitude of the change.

We now use the theory of random walks to provide a geometrical interpretation of the shift in T_c of order $1/n^2$ since this will help us to consider the analogous problem for a SAW. We have dealt with a particle describing a random walk in a finite slab consisting of $n(d - 1)$ layers in d dimensions. At each point the particle has $(2d)$ possible choices except at the boundary where it has only $(2d - 1)$ choices. We are concerned with a long walk in which the particle diffuses forwards and backwards m times between the boundaries, and each transition from one boundary to the other takes M steps ($N = mM$). From diffusion theory we know that

$$n \sim aM^{1/2}. \quad (23)$$

The total number of walks is then of the order

$$\{(2d)^{M-1}(2d-1)\}^m = (2d)^N \left(1 - \frac{1}{2d}\right)^{N/M} = (2d)^N \left(1 - \frac{1}{2dM}\right)^N \quad (24)$$

so that the new effective coordination number is

$$2d - \frac{a^2}{n^2}. \quad (25)$$

This is in agreement with (17).

3. Perturbation treatment of random walks

The idea of introducing a repulsive interaction between pairs of steps of a random walk and hence making a transition from a random walk to a SAW was first put forward by Brout (1961) and has been developed recently by Domb and Joyce (1972). Brout showed that a certain class of diagrams (termed 'ladder diagrams' by Domb and Joyce) could be summed in closed form and yielded the spherical model solution. There is theoretical evidence to suggest that in high dimensions ($d \geq 4$) the non-ladder diagrams cease to play a significant role, and the ladder approximation is close to the true solution. We should emphasize that the above agreement with the spherical model is *formal* in character; we are in fact dealing with an approximation to SAW and not with a set of lattice spins satisfying the spherical model condition (Joyce 1972). We may take as an illustrative parallel the Bethe approximation and the solution for a 'Bethe' lattice (Domb 1960 p 284). Although these two give the same result for bulk free energy their surface properties are quite different. Thus although some of our results may agree with those of Fisher and Barber (1972) for the spherical model, we should not be surprised to find that some of them differ.

Domb and Joyce introduced an interaction $w\delta_{ij}$ between each pair of points of a random walk which occupied sites i and j of the lattice. A perturbation expansion was developed in powers of w , $w = -1$ corresponding to the SAW. The ladder diagrams could all be expressed in terms of the generating function for random walk returns

to the origin :

$$R(x) = \sum_{n=2}^{\infty} \frac{u_N}{c_N} x^N = e(x) + f(x)(1-x)^2 \tag{26}$$

where

$$e(x) = e_0 + e_1(1-x) + e_2(1-x)^2 + \dots \tag{27}$$

Domb and Joyce found that if we denote the new value of c_N by

$$c_N(w) \sim (\mu(w))^N \tag{28}$$

then $\mu(w)$ depends on e_0 only.

When we introduce a cyclic boundary into the problem, we introduce the possibility of new contacts after 1, 2, 3, ... loops of the torus. This means that $R(x)$ must be replaced by

$$R(x) + 2(R_n(x) + R_{2n}(x) + R_{3n}(x) + \dots), \tag{29}$$

where $R_{sn}(x)$ corresponds to contacts after looping the torus s times. Now

$$R_n(x) = \sum_{N=n}^{\infty} \frac{c_N(n, \mathbf{0})}{c_N} x^N \tag{30}$$

using the same notation as in (21). The function $R_n(x)$ is well known (Joyce 1972, Montroll and Weiss 1965) as

$$\frac{1}{n^{d-2}} F(n(1-x)^{1/2}) \tag{31}$$

where the function F tends to a finite limit as $x \rightarrow 1$. In fact we require only the analogue of e_0 ($= (R(1))$) which is

$$R_n(1) = \frac{B}{n^{d-2}}. \tag{32}$$

Similarly for $R_{sn}(x)$. Hence in the ladder approximation e_0 is replaced by

$$e_0 + \frac{B}{n^{d-2}} \left(1 + \frac{1}{2^{d-2}} + \frac{1}{3^{d-2}} + \dots + \frac{1}{s^{d-2}} + \dots \right). \tag{33}$$

The series converges as long as $d \geq 4$. Hence as long as $d \geq 4$ this finite size effect is of order $1/n^{d-2}$. This is the same as the result obtained by Fisher and Barber (1972) for the spherical model with cyclic boundaries.

We can understand geometrically why this finite size effect is dimension dependent. Let us consider a particle diffusing in d dimensional space. When we put the particle on a torus we must eliminate all contacts which arise because the particle has looped the torus. These will be represented by the 'overlap' with the original distribution of walks which have remained in the same position in the d th dimension after traversing n layers of the lattice. However, the walks will have diffused in the remaining $(d-1)$ dimensions, and the larger the value of d the smaller the overlap.

For a finite strip we may also expect a finite size effect comparable to the above, corresponding to the overlap of walks after reflection from the boundary. As long as $d > 4$ this finite size effect is of less significance than the effect of the free boundary. When $d = 4$ the two effects are of comparable size.

We note that when $d = 3$ the series (33) diverges, and this means that the non-ladder diagrams now play a fundamental role. Since these diagrams are complex and difficult to analyse we adopt an alternative starting point of free SAW in three dimensions. The discussion must now be more qualitative, but we hope that we can obtain a heuristic idea of the magnitude of the two effects described above.

4. Self-avoiding walks in three dimensions

When we pass from a random walk to a self-avoiding walk the total number of walks and their space distribution both change. For example c_N and u_N become

$$\begin{aligned} c_N &\sim \mu^N N^g \\ u_N &\sim \mu^N N^{-h} \end{aligned} \tag{34}$$

where μ is the new 'effective coordination number', and g and h are exponents which differ from the random walk values in three dimensions ($g = 0, h = \frac{3}{2}$). Similarly the mean square end-to-end length of the walk becomes

$$\langle R_N^2 \rangle \sim N^{2\nu}, \tag{35}$$

where ν is approximately (and possibly exactly) $\frac{3}{5}$ instead of $\frac{1}{2}$, which corresponds to a random walk. A SAW can conveniently be related to a diffusion process in the presence of a potential (Edwards 1965).

If we now try to estimate the effect of a finite barrier we can use the same diffusion argument as at the end of § 2, but instead of (23) we have

$$n \sim aM^\nu. \tag{36}$$

The total number of walks is then of the order

$$\{\mu^{M-1}(\mu-b)\}^m = \mu^N \left(1 - \frac{b}{\mu}\right)^{N/M} = \mu^N \left(1 - \frac{b}{\mu^M}\right)^N, \tag{37}$$

so that the new effective coordination number is now

$$\mu - b \left(\frac{a}{n}\right)^{1/\nu}. \tag{38}$$

Interpreting (38) for the Ising model we find that the barrier itself produces a lowering of critical temperature of order n^{-1/ν_3} where ν_3 is the three dimensional correlation exponent (Fisher 1967). This has the form of Fisher's estimate (1971).

To deal with a cyclic barrier we follow the perturbation procedure described in § 3, introducing an interaction $w\delta_{ij}$ between each pair of points of the SAW, and putting $w = -1$ to eliminate all walks which cease to be self-avoiding after looping the torus. The perturbation diagrams are exactly the same as described by Domb and Joyce (1972), but because of the self-avoidance condition different sections of the walk are no longer independent, and therefore the expression of these diagrams in terms of products of generating functions is no longer correct. Nevertheless since the only interactions correspond to walks a great distance apart, it is reasonable to expect that the generating function description will give an estimate of the order of magnitude of the various terms.

We use an asterisk to denote the analogues of the functions in (29). Since there are no direct contacts

$$R^*(x) = 0. \tag{39}$$

Instead of (31) we have for SAW (Domb 1970)

$$R_n^*(x) = \frac{1}{n^{d-2+\eta}} F(n(1-x)^\nu) \tag{40}$$

where η (Fisher 1967) is small but greater than zero (about $\frac{1}{8}$ in three dimensions); thus the value of $R_n^*(1)$ is—instead of (32)—

$$R_n^*(1) \simeq \frac{B^*}{n^{1+\eta}}. \tag{41}$$

In the ladder approximation we have

$$e_0^* \simeq \frac{B^*}{n^{1+\eta}} \left(1 + \frac{1}{2^{1+\eta}} + \frac{1}{3^{1+\eta}} + \dots \right) \tag{42}$$

where the sum on the right-hand side of (42) now converges.

From (42) we see that the first-order term in the expansion in powers of e_0^* is the most important, and is of order $n^{-1-\eta}$. There is evidence that non-ladder terms which involve at least two contacts will be of order $n^{-2-2\eta}$.

Our analysis therefore leads to the suggestion that in three dimensions a finite size effect of order $n^{-1-\eta}$ may be more important than the presence of a finite barrier. For a torus this is the only effect present, whereas for a finite strip there is an additional effect of order n^{-1/ν_3} . This suggestion is put forward only tentatively and we hope to undertake a program of numerical studies of SAW to provide a better basis for an assessment.

The numerical estimates of Allan (1970) discussed in the introduction seem to lead to a different conclusion. However, we wish to point out that for a torus each successive looping produces a marked effect, and successive effects diminish rather slowly. In considering the 12th term of a susceptibility series, for example, $n = 3$ allows four loops of the torus, whereas $n = 7$ or 8 allow only one. Thus for lower values of n a larger proportion of the total contribution has been taken into account than for higher values of n , and the convergence in n has been artificially accelerated. A similar type of effect might also be expected to occur with a finite strip, but it is more difficult to disentangle the various contributions in this case. The extrapolation procedure would be more reliable if the contributions of successive loops of the torus could be kept separate; we hope to undertake numerical calculations for SAW taking this into account.

We may also note that recent exact calculations for finite systems by Binder (1972) have suggested that the shift in critical temperature in three dimensions may be of order n^{-1} .

5. Conclusions

It is suggested that there are two independent effects which determine the deviation in critical temperature of an n layer ($d - 1$) dimensional Ising system from the bulk d dimensional value: (i) the finite size effect of order $1/n^{d-2+\eta}$; (ii) the effect of free boundaries

of order $1/n^{1/\nu}$. When $d \geq 4$ the deviation is of order $1/n^2$ for a free boundary, and of order $1/n^{d-2}$ for a cyclic boundary. When $d = 3$ the deviation is of order $1/n^{1+\eta}$ for both types of boundary, but the free boundary has an extra term of order $1/n^{1/\nu}$.

Certain of the above features are in agreement with the results of Fisher and Barber (1972) for the spherical model. The most significant difference is in the value of λ for a free surface which the above authors find to be 1.

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