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Critical temperature shifts for finite slabs in the ϵ-expansion

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Abstract. The critical temperature $T_c(b)$ of a d-dimensional system with finite thickness b in one of its dimensions approaches its bulk limit as $b \to \infty$ according to $T_c(\infty) - T_c(b) \propto b^{-\lambda}$. To first order in $\epsilon = 4 - d$ the shift exponent λ is found to be given by $\lambda = 2 - [(n+2)/(n+8)]\epsilon + O(\epsilon^2)$, and thus satisfies the scaling relation $\lambda = \nu_d^{-1}$, where ν_d is the correlation length exponent of the bulk system and n is the order parameter dimensionality.

1. Introduction

The renormalisation group and the associated techniques of expansion in powers of $\epsilon = 4 - d$ and $1/n$, where d is the spatial dimensionality and n the 'spin dimensionality' of the system, have proved to be powerful tools in the study of the critical behaviour of bulk systems (Ma 1973, 1976, Fisher 1974, Wilson and Kogut 1974). More recently the same techniques have been applied to the critical behaviour of semi-infinite systems (Lubensky and Rubin 1973, 1975, Bray and Moore 1977a, b, c). In the present paper we use the ϵ-expansion to investigate the critical behaviour of films which are infinite in $(d-1)$ spatial dimensions, but have finite thickness b in the remaining dimension.

Two critical exponents characterise the critical behaviour of such films in the limit $b \to \infty$ (Fisher and Barber 1972, Barber 1973, Fisher 1973). The 'shift' exponent λ describes the b-dependence of the transition temperature, $T_c(\infty) - T_c(b) \propto b^{-\lambda}$. The 'rounding' exponent θ characterises the 'crossover' from d-dimensional to $(d-1)$-dimensional critical behaviour as $t = (T - T_c)/T_c$ decreases, the crossover occurring at $t \approx t^* \propto b^{-\theta}$. Intuitively, one expects this crossover to occur when the bulk correlation length ξ $(\propto t^{-\nu_d})$ exceeds the film thickness b, which yields $\theta = 1/\nu_d$ (Fisher and Ferdinand 1967, Ferdinand and Fisher 1969). This scaling result, which may be derived more formally by writing the crossover function in scaling form (Fisher and Barber 1972, Barber 1973) is generally accepted as valid. Concerning the value of the shift exponent λ, however, there seems to be less general agreement. Simple scaling arguments (Fisher and Barber 1972) yield $\lambda = \theta = 1/\nu_d$ and this result is supported by high temperature series expansion (Fisher 1971) and Monte Carlo simulations (Binder and Hohenberg 1974). On the other hand, exact solution of the spherical model (Fisher and Barber 1972, 1973) gives $\lambda = 1$ in all dimensions, while recent rather precise experimental work on helium films near T_λ (Chen and Gasparini 1977) suggests that for this case $\lambda^{-1} \simeq 0{\cdot}56 < \nu_d$.

Against the background of this uncertainty it would seem useful to have an explicit calculation of λ within the ϵ-expansion. Such a calculation is carried out here and

yields $\lambda = 2-[(n+2)/(n+8)]\epsilon + O(\epsilon^2)$, consistent with the scaling prediction $\lambda = \nu_d^{-1}$. The calculation makes use of the Wilson (1972) perturbation theory technique. Section 2 is devoted to a brief resumé of the mean field theory calculation of λ (Kaganov and Omelyanchouk 1971, Wolfram *et al* 1971), the result being a starting point for the ϵ-expansion. In § 3, the mean field theory result is recovered using the 'eigenvalue method', a technique well suited for use in connection with the ϵ-expansion. The order ϵ contribution to λ is computed in § 4, while § 5 concludes with a discussion of the result.

2. Mean field theory

We adopt the conventional Ginzburg–Landau–Wilson model Hamiltonian,

$$H = \int \mathrm{d}^d x \left[\tfrac{1}{2} r_0 \sum_i \phi_i^2 + \tfrac{1}{2} \sum_i (\nabla \phi_i)^2 + \frac{u}{4} \left(\sum_i \phi_i^2 \right)^2 \right], \tag{2.1}$$

with partition function $Z = \int D\phi \exp(-H)$. The integral in equation (2.1) extends over the region between the planes $z = -b/2$ and $z = b/2$, $\boldsymbol{\phi} = (\phi_1, \ldots, \phi_n)$ is the n-component order parameter, and $r_0 \propto (T - T_c^0(\infty))$. Above its critical point T_c^0 mean field theory amounts to neglecting the term in u in equation (2.1). The order parameter correlation function is $G(\boldsymbol{x}, \boldsymbol{x}') = \langle \phi_i(\boldsymbol{x}) \phi_i(\boldsymbol{x}') \rangle$ where angular brackets represent a thermal average and $G(\boldsymbol{x}, \boldsymbol{x}')$ is independent of i from the isotropy of the model. In mean field theory $G(\boldsymbol{x}, \boldsymbol{x}')$ satisfies the linear differential equation (Mills 1971)

$$-\nabla^2 G(\boldsymbol{x}, \boldsymbol{x}') + r_0 G(\boldsymbol{x}, \boldsymbol{x}') = \delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{2.2}$$

For simplicity we adopt boundary conditions $G(\boldsymbol{x}, \boldsymbol{x}') = 0$ at $z = \pm b/2$, which is a special case of the 'extrapolation length' type of boundary condition (Mills 1971, Binder and Hohenberg 1972), $(\partial/\partial z) G(\boldsymbol{x}, \boldsymbol{x}') = \pm l^{-1} G(\boldsymbol{x}, \boldsymbol{x}')$ for $z = \mp b/2$, with the extrapolation length l equal to zero. Provided $l \geqslant 0$ the critical exponents are expected to be independent of the value of l and this is easily verified within mean field theory. Our choice of boundary condition corresponds to a boundary condition on the order parameter: $\phi_i(\boldsymbol{x}) = 0$ for $z = \pm b/2$.

It is convenient to make use of the translational invariance parallel to the slab. To this end we write $\boldsymbol{x} = (\boldsymbol{\rho}, z)$ with $\boldsymbol{\rho}$ a $(d-1)$-dimensional vector parallel to the film surfaces, and express $G(\boldsymbol{x}, \boldsymbol{x}')$ as the Fourier sum $G(\boldsymbol{x}, \boldsymbol{x}') = \Sigma_{\boldsymbol{k}} G_{\boldsymbol{k}}(z, z') \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}')]$, where

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2} + r_0 + k^2 \right) G_{\boldsymbol{k}}(z, z') = \delta(z - z'). \tag{2.3}$$

With the boundary condition $G_{\boldsymbol{k}}(\pm b/2, z') = 0$, the solution of equation (2.3) is

$$G_{\boldsymbol{k}}(z, z') = \frac{\sinh \kappa(\frac{1}{2}b - z') \sinh \kappa(\frac{1}{2}b + z)}{\kappa \sinh \kappa b}, \qquad z < z' \tag{2.4}$$

where

$$\kappa = (r_0 + k^2)^{1/2}. \tag{2.5}$$

For $z > z'$ the same result, equation (2.4), holds, but with z and z' interchanged.

As the temperature is lowered, i.e. r_0 is decreased, the first singularity in $G_{\boldsymbol{k}}(z, z')$ occurs at the first non-trivial zero of $\sinh \kappa b$, namely, at $\kappa b = \pi \mathrm{i}$. Thus the $\boldsymbol{k} = 0$ mode first becomes critical, at a temperature r_{0c} given by

$$r_{0c} = -\pi^2/b^2. \tag{2.6}$$

Thus in mean field theory one has $\lambda = 2$, in agreement with the scaling prediction $\lambda = \nu_d^{-1}$ since $\nu_d = \frac{1}{2}$ in mean field theory.

3. The eigenvalue method

This is an alternative, simpler, technique for the determination of the critical temperature. Neglecting as before the term in u in equation (2.1), and introducing the Fourier components of the order parameter via $\phi_i(\boldsymbol{\rho}, z) = \Sigma_{\boldsymbol{k}} \phi_i(\boldsymbol{k}, z) \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{\rho})$, the Hamiltonian may be written, using integration by parts, as

$$H = \tfrac{1}{2} \int_{-b/2}^{b/2} \mathrm{d}z \sum_{i,\boldsymbol{k}} \phi_i(-\boldsymbol{k}, z)\left(-\frac{\mathrm{d}^2}{\mathrm{d}z^2} + r_0 + k^2\right)\phi_i(\boldsymbol{k}, z) \tag{3.1}$$

where the boundary conditions $\phi_i(\boldsymbol{k}, \pm b/2) = 0$ were used to eliminate the surface terms. Writing the operator in large parentheses in equation (3.1) as L we introduce its (real) eigenfunctions ψ_α and eigenvalues μ_α,

$$L\psi_\alpha = \mu_\alpha \psi_\alpha, \tag{3.2}$$

where the $\psi_\alpha(z)$ satisfy the boundary conditions $\psi_\alpha(\pm b/2) = 0$. Expanding the order parameter as

$$\phi_i(\boldsymbol{k}, z) = \sum_\alpha a_{i\alpha}(\boldsymbol{k}) \psi_\alpha(z) \tag{3.3}$$

yields

$$H = \tfrac{1}{2} \sum_{i,\alpha,\boldsymbol{k}} \mu_\alpha a_{i\alpha}(\boldsymbol{k}) a_{i\alpha}(-\boldsymbol{k}) \tag{3.4}$$

so that the expansion coefficients $a_{i\alpha}(\boldsymbol{k})$ have correlation functions

$$\langle a_{i\alpha}(\boldsymbol{k}) a_{j\beta}(-\boldsymbol{k}')\rangle = \delta_{\boldsymbol{k},\boldsymbol{k}'}\, \delta_{i,j}\, \delta_{\alpha,\beta}/\mu_\alpha. \tag{3.5}$$

The critical point occurs when the smallest eigenvalue becomes zero. Hence to determine the shift exponent we require only the smallest eigenvalue of the operator L and need not calculate the entire function $G_{\boldsymbol{k}}(z, z')$. This will be an immense simplification in computing the shift exponent to order ϵ. Note, however, that $G_{\boldsymbol{k}}(z, z')$ may be recovered from the complete set of eigenvalues and eigenfunctions:

$$G_{\boldsymbol{k}}(z, z') = \langle \phi_i(\boldsymbol{k}, z) \phi_i(-\boldsymbol{k}, z')\rangle$$

$$= \sum_{\alpha,\beta} \psi_\alpha(z) \psi_\beta(z') \langle a_{i\alpha}(\boldsymbol{k}) a_{i\beta}(-\boldsymbol{k})\rangle = \sum_\alpha \mu_\alpha^{-1} \psi_\alpha(z) \psi_\alpha(z'). \tag{3.6}$$

The eigenfunctions of the operator $L = (-\mathrm{d}^2/\mathrm{d}z^2) + r_0 + k^2$ which satisfy the boundary conditions $\psi(\pm b/2) = 0$ are

$$\psi_n(z) = \begin{cases} (2/b)^{1/2} \cos(n\pi z/b), & n = 1, 3, 5, 7, \ldots \\ (2/b)^{1/2} \sin(n\pi z/b), & n = 2, 4, 6, 8, \ldots . \end{cases} \tag{3.7}$$

The corresponding eigenvalues are

$$\mu_{n,k} = r_0 + k^2 + (n\pi/b)^2, \qquad n = 1, 2, 3, 4, \ldots \tag{3.8}$$

The smallest eigenvalue is $\mu_{1,0} = r_0 + (\pi/b)^2$ giving the location of the critical point as

$$r_{0c} = -\pi^2/b^2 \tag{3.9}$$

as before. The eigenfunction corresponding to the smallest eigenvalue is

$$\psi_1(z) = (2/b)^{1/2} \cos(\pi z/b). \tag{3.10}$$

4. Shift exponent to order ϵ

To calculate the $O(\epsilon)$ contribution to the shift exponent we will use the Wilson (1972) perturbation theory technique. This involves expanding to first order in the coupling constant u, which is then set equal to a special value u_w chosen to eliminate the leading correction to scaling. The singular part of the free energy (for example) is expected to have the form

$$F(t, h, b) = t^{2-\alpha} f_1(ht^{-\Delta}, bt^{1/\lambda}) + (u - u_w) t^{2-\alpha+\omega} f_2(ht^{-\Delta}, bt^{1/\lambda}) + \ldots, \tag{4.1}$$

where h is a uniform magnetic field (included for generality), Δ is the gap exponent, $\omega = O(\epsilon)$ is the correction-to-scaling exponent and t measures the deviation from the bulk critical temperature. In equation (4.1) u_w is a constant, independent of all the 'fields' $t, h, b^{-1}, \ldots$ in the problem. It has the value $u_w = 8\pi^2\epsilon/(n+8) + O(\epsilon^2)$ (Wilson 1972). Setting $u = u_w$ eliminates the leading correction to scaling and thereby makes possible unambiguous exponentiation of logarithms.

First-order perturbation theory is equivalent to including a potential term $V(z)$ in the operator L, where

$$V(z) = u(n+2) \sum_{k<\Lambda} G_k(z, z).$$

Here $(n+2)$ is the usual combinatoric factor associated with the one loop graph of first-order perturbation theory, and Λ is a large momentum cut-off for momenta parallel to the slab. Use of equation (2.4) yields

$$V(z) = u(n+2) \sum_{k<\Lambda} \frac{\cosh(\kappa b) - \cosh(2\kappa z)}{2\kappa \sinh \kappa b} \tag{4.2}$$

where $\kappa = (r_0 + k^2)^{1/2}$ as usual. The $O(u)$ contribution to the lowest eigenvalue $\mu_{1,0}$ is

$$\delta\mu_{1,0} = \int_{-b/2}^{b/2} dz\, \psi_1^2(z) V(z)$$

$$= \frac{u(n+2)}{b} \sum_{k<\Lambda} \frac{1}{\kappa \sinh \kappa b} \int_{-b/2}^{b/2} dz \cos^2\left(\frac{\pi z}{b}\right) [\cosh(\kappa b) - \cosh(2\kappa z)]. \tag{4.3}$$

The integral over z is straightforward and yields

$$\delta\mu_{1,0} = \frac{u(n+2)b}{2} \sum_{k<\Lambda} \left(\frac{\coth \kappa b}{\kappa b} - \frac{\pi^2}{(\kappa b)^2[(\kappa b)^2 + \pi^2]} \right). \tag{4.4}$$

The implicit equation which determines the critical value of r_0 is

$$\mu_{1,0} = r_0 + (\pi/b)^2 + \delta\mu_{1,0} = 0. \tag{4.5}$$

To lowest order in u we may, however, set $r_0 = -\pi^2/b^2$ in evaluating $\delta\mu_{1,0}$. Therefore, to order u, the critical value of r_0 is

$$r_{0c} = (-\pi^2/b^2) - \delta\mu_{1,0}(r_0 = -\pi^2/b^2). \tag{4.6}$$

In equation (4.4) we may therefore write $\kappa^2 = k^2 - \pi^2/b^2$ to give

$$\delta\mu_{1,0} = \frac{u(n+2)b}{2} \sum_{k<\Lambda} \left(\frac{\coth(b^2k^2 - \pi^2)^{1/2}}{(b^2k^2 - \pi^2)^{1/2}} - \frac{\pi^2}{(b^2k^2 - \pi^2)b^2k^2} \right). \tag{4.7}$$

Fortunately, it is only necessary to extract the leading logarithm (i.e. a term in $b^{-2} \ln b$) from this integral. The second term in the large parentheses produces no logarithms (the singularity at $k = \pi/b$ is exactly cancelled by that in the first term). The logarithm comes from the behaviour of the first term when $kb \gg 1$, in which régime $\coth(b^2k^2 - \pi^2)^{1/2}$ may be replaced by unity (corrections are exponentially small). Hence to logarithmic accuracy,

$$\delta\mu_{1,0} = \frac{u(n+2)}{2} \sum_{k<\Lambda} \frac{1}{k} \left(1 - \frac{\pi^2}{b^2k^2}\right)^{-1/2} = \frac{u(n+2)}{2} \sum_{k<\Lambda} \frac{1}{k} \left(1 + \frac{\pi^2}{2b^2k^2} + \ldots\right). \tag{4.8}$$

The first term in the bracket leads to the standard $O(u)$ shift in the bulk critical temperature, $u(n+2)\Sigma_{k<\Lambda} 1/2k = \delta r_{0c}^{\text{bulk}}$. The second term leads to the desired logarithm. Since u will eventually be set equal to $u_w = O(\epsilon)$, the sum over $\boldsymbol{k}$ may be evaluated in three dimensions. The resulting logarithmic divergence at small k is cut-off at $k \sim b^{-1}$, since the expansion in equation (4.8) is only valid for $kb \gg 1$. To logarithmic accuracy, then, we find

$$\delta\mu_{1,0} = \delta r_{0c}^{\text{bulk}} + \frac{u(n+2)}{8b^2} \ln(b\Lambda). \tag{4.9}$$

Substituting in equation (4.6) and choosing $u = u_w = 8\pi^2\epsilon/(n+8) + O(\epsilon^2)$ yields

$$\begin{aligned} r_{0c} &= -\delta r_{0c}^{\text{bulk}} - \frac{\pi^2}{b^2}\left[1 + \epsilon\left(\frac{n+2}{n+8}\right) \ln(b\Lambda)\right] + O(\epsilon^2) \\ &= -\delta r_{0c}^{\text{bulk}} - \frac{\pi^2}{b^2}(b\Lambda)^{[(n+2)/(n+8)]\epsilon} + O(\epsilon^2). \end{aligned} \tag{4.10}$$

Hence the shift exponent is

$$\lambda = 2 - \left(\frac{n+2}{n+8}\right)\epsilon + O(\epsilon^2), \tag{4.11}$$

an expansion identical to that of ν_d^{-1}.

5. Discussion

The order ϵ result presented here lends strong support to the scaling prediction $\lambda = \nu_d^{-1}$.

In the limit $n \to \infty$ one obtains $\lambda = 2 - \epsilon + O(\epsilon^2)$ in contrast to the spherical model result $\lambda = 1$ for all d. While this may seem surprising at first sight, one must remember that the correspondence (Stanley 1968) between the spherical model and the $n = \infty$ limit of the n-vector model only holds for bulk systems. For systems lacking translational invariance in one direction, the $n = \infty$ limit probably corresponds to a spherical model with a separate spherical constraint on every layer. The shortcomings of the single constraint spherical model have recently become clear in connection with the semi-infinite problem (Bray and Moore 1977a, c).

The discrepancy between the scaling prediction and the experimental results of Chen and Gasparini (1977) seems harder to understand. These authors have measured the specific heat of helium at the λ transition for films of various thickness and filled channels of various diameters. By measuring the location of the specific heat maximum as a function of film thickness or channel size they are able to determine the shift exponent (Moore 1971). The result is $\lambda^{-1} = 0{\cdot}562 \pm 0{\cdot}014$, compared to a value $\nu_d = 0{\cdot}675 \pm 0{\cdot}001$ deduced from the result for the bulk specific heat exponent α_d and use of the hyperscaling relation $2 - \alpha_d = d\nu_d$. Should this discrepancy be confirmed in subsequent work, it would seem worthwhile to attempt the very much harder $O(\epsilon^2)$ calculation of the shift exponent.

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