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LETTER TO THE EDITOR

The Ising model below T_c: calculation of non-universal amplitudes using a primitive droplet model

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Abstract. Using recent exact results for the surface free energies of Ising droplets on a square lattice, and applying a primitive droplet theory due to Langer, we obtain an expression for the principal non-universal amplitude appearing in the imaginary part of the analytic continuation of the free energy across the coexistence line for the square lattice Ising model below T_c. The significance of this calculation is the known dependence on this amplitude of the large-order terms in the expansion of the physical free energy in powers of H, thus allowing a direct numerical comparison with existing series data to be made. After carrying out a simple renormalisation of the droplet volume term, we find excellent numerical agreement.

The work of Langer (1967) and Gunther *et al* (1980) provides strong evidence that the analytic continuation of the free energy $F(H)$ of a d-dimensional Ising model below T_c in a field $H>0$, into the complex H plane, has a branch cut singularity at the origin. If the branch cut is drawn along the negative H axis Re $F(H)$ is continuous across the cut, while Im $F(H)$ takes the following form for small $|H|$

$$\text{Im } F(e^{\pm i\pi}|H) = \mp B|H|^b \exp -\{A|H|^{-a}[1+O(H^2)]\}. \tag{1a}$$

A and B are non-universal constants, while the powers a and b, which have been determined explicitly, are universal, at least in 2D. In fact (Gunther *et al* 1980)

$$a = d-1 \tag{1b}$$

$$b = \tfrac{1}{2}(3-d)d, \qquad 1<d<5 \qquad d\neq 3$$

$$= -\tfrac{7}{3}, \qquad d=3. \tag{1c}$$

The asymptotic form of high-order coefficients in the physical free energy $F(H)$, $H>0$, and its derivatives, in powers of H, can be obtained from (1) via a dispersion relation (Gunther *et al* 1980—see also Wallace 1978). This feature has been used by Lowe and Wallace (1980), henceforth denoted by LW, to test the result (1) in two dimensions; this was done by comparing with long series in H for the magnetisation, at a fixed temperature well below T_c, due to Baker and Kim (1980), hereafter denoted by BK. Explicitly, BK obtain series of the form

$$\tilde{M} \sim \sum_{L=0} \tilde{M}_L(-2H)^L \tag{2}$$

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for the Ising model at subcritical temperatures on various lattices. Here $\tilde{M} = \frac{1}{2}(1-M)$ where M is the magnetisation. The series (2) were obtained by an integral approximant analysis of the low-temperature series expansion work of Baxter and Enting (1979) and Sykes *et al* (1973, 1975). For the particular case of the square lattice, (2) was obtained to 24th order at a temperature $\exp(-4\beta_1 J) = 0.1\exp(-4\beta_c J)$ and to 12th order at temperature $\exp(-4\beta_2 J) = 0.9\exp(-4\beta_c J)$. The high-order estimate calculation, starting from (1), is carried out in LW and yields the following result in two dimensions

$$b_L = (1/2A)[1 + (1-b)L^{-1} + O(L^{-2})] \tag{3}$$

where $b_L = \tilde{M}_L / L\tilde{M}_{L-1}$.

Using only the BK data at the lower temperature LW note that the stabilisation of the b_L towards a constant value as L increases is fairly convincing, and their analysis of the data further suggests that the coefficient of L^{-1} in (3) is zero, consistent with the 2D value of $b = 1$ from (1*c*), thus making more precise the original conclusions of BK concerning the asymptotic nature of the series (2). However, as remarked by LW, the results (1) were obtained using the standard ϕ^4 field theory which, though in the same universality class as the Ising model, does not yield the value of the non-universal constant A.

The purpose of the present letter is to point out that the primitive droplet theory of Langer (1967)—see also Fisher (1967)—which starts from the classical lattice droplet model, and was developed as a precursor of the field theory, contains an explicit expression for A in terms of a lattice-dependent parameter, namely the surface free energy of an equilibrium Ising droplet of unit volume. We then use the recent work of Zia and Avron (1982), in which exact results for this last quantity are obtained on a square lattice, for a numerical calculation of A, so that comparison with the BK data, and hence a further test of the result (1), can be made.

The classical droplet model has as its starting point an Ising model well below T_c, so that nearly all the spins are up (say) and the regions of down spins can be considered as a dilute gas of non-interacting clusters. The number of clusters per site of size l is then given by a simple Boltzmann distribution $\exp(-\beta\phi_l)$ where ϕ_l is the free energy of an l-site cluster. ϕ_l is assumed to take the following form for large l:

$$\phi_l = 2M\beta^{-1}Hl + \Sigma l^{(d-1)/d} \tag{4}$$

The first term on the RHS of (4) is the droplet volume term and, in the original droplet model in which the factor M is omitted, is just the energy required to flip all l spins of the droplet in the reduced magnetic field H. The inclusion of the factor M, the magnetisation, in the droplet volume term incorporates the effect of droplet nesting, which becomes increasingly important as T increases from zero to T_c. This is because the effect of droplet nesting is to reduce the fraction of overturned spins in a large minority droplet from 1 to M. Here 'large' means that the linear dimension of the droplet must be much greater than both the lattice spacing and the thermal correlation length. The second term in (4) represents the free energy of the droplet boundary separating the regions of up and down spins. This is proportional to the surface area of the droplet which is assumed to be compact (with surface area $\propto$ (volume)$^{(d-1)/d}$) but whose shape is otherwise unspecified in (4). Σ is therefore the surface free energy of an equilibrium droplet of unit volume. The droplet free energy (4), with its *ad hoc* renormalisation of the droplet volume energy, has been used recently by Binder (1983) in a continuum treatment of nucleation free energy barriers near T_c, while again near

T_c and in the continuum, the form (4) is made respectable in $1+\varepsilon$ dimensions by the droplet theory of Bruce and Wallace (1983)—see also Bruce and Sim (1983). Here, we emphasise that we shall assume the literal validity of the simple droplet model with free energy given by (4) on the lattice and over the entire temperature range $[0, T_c]$. We remark that although this model incorporates one of the effects of the non-diluteness of the droplet gas as T approaches T_c, droplet nesting, the cluster–cluster interactions resulting from overlapping droplet boundaries are neglected. However, the former effect appears to be the dominant one in two dimensions. According to the above model, the free energy per site of the system is given by

$$F(H) = -\frac{H}{\beta} + \frac{1}{\beta}\sum_{l=1}^{\infty} \exp -\beta\phi_l \tag{5}$$

$$\sim -\beta^{-1}H + \frac{d}{\beta}(\beta\Sigma)^d(2MH)^{-d}$$

$$\times \int_0^{\infty} \mathrm{d}t\, t^{d-1} \exp -\{(\beta\Sigma)^d(2MH)^{-(d-1)}(t^d + t^{d-1})\}. \tag{6}$$

Substitution of (4) into (5), replacement of the sum by an integral, followed by a change of variable, yields the expression (6), which is valid for small H. The analytic continuation of (6) from real positive H into the complex H plane is straightforward, and has been carried out by Langer (1967) for $d=3$. One finds that $F(H)$ has a branch point at $H=0$, and if the branch cut is drawn along the negative H axis, a result of the form (1*a*) is obtained, with

$$a = d-1, \qquad A = \frac{(\beta\Sigma)^d(d-1)^{(d-1)}}{2^{d-1}d^dM^{d-1}} \tag{7a}$$

$$-b = \tfrac{1}{2}(d+1), \qquad B = \frac{d}{2\beta}\left\{\frac{(d-1)^d\pi(\beta\Sigma)^d}{M^{d-1}2^dd^{d+1}}\right\}^{1/2}. \tag{7b}$$

The leading term in the exponential of (1*a*) has a physical interpretation as $\beta\times$ the free energy ϕ_{lc} of the critical droplet of size l_c which maximises ϕ_l for $H<0$. This interpretation also carries over to the field theoretic treatment leading to (1), whose additional inclusion of droplet shape fluctuations accounts for the difference in the results (1*c*) and (7*b*) for the exponent b (Langer 1967).

It is our present purpose to test the critical droplet picture by evaluating the quantity $1/2A$ using the expression (7*a*) for the principal non-universal amplitude A, and comparing with the corresponding values of b_∞ estimated from the square lattice. The estimates of b_∞ at the two temperatures β_1 and β_2 were obtained by plotting values of b_L, calculated from the BK data, against $1/L^2$ and using the fact that the plots should approach a straight line for large L. These plots, together with the corresponding estimates of b_∞ are displayed in figure 1. In order to compare with $1/2A$, we require numerical values for the surface free energy Σ at the two temperatures β_1 and β_2. We use the following results, taken from Zia and Avron (1982)

$$\Sigma = dW^{1/d} \tag{8}$$

where W is the volume of the Wulff construction

$$R(\hat{r}) = \min_{\hat{n}}\sigma(\hat{n})/(\hat{n}\cdot\hat{r}) \tag{9}$$

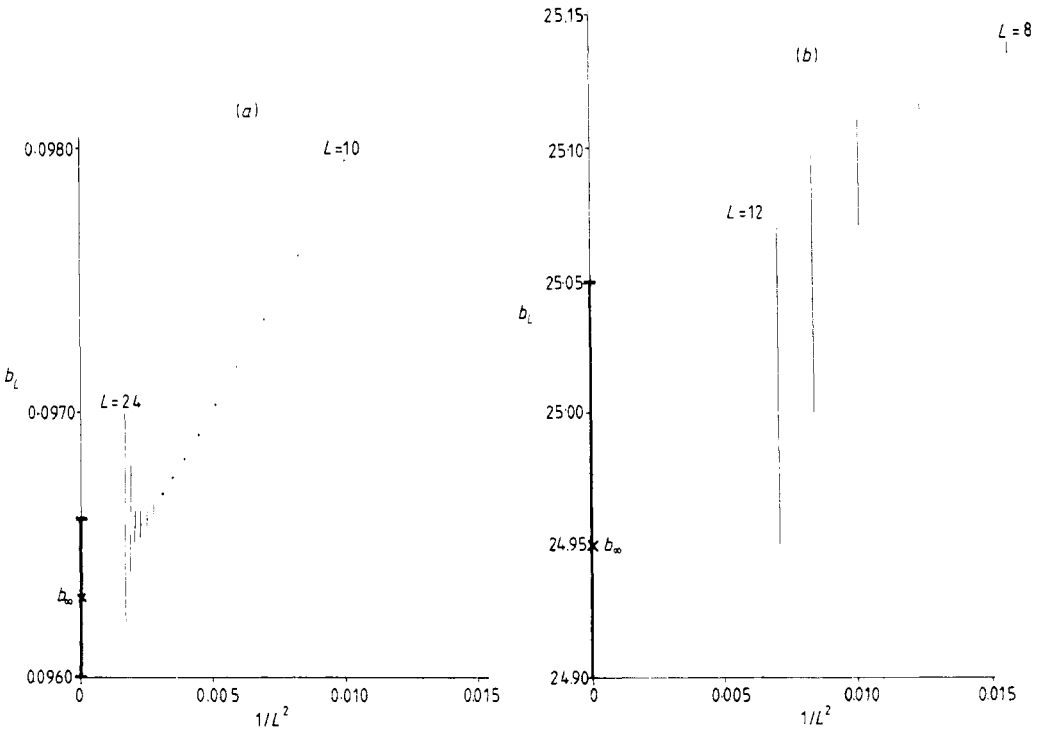

Figure 1. Plots of $b_L = \tilde{M}_L / L\tilde{M}_{L-1}$ against $1/L^2$ using the square lattice $\tilde{M}_L$ data of Baker and Kim (1980) at temperatures (*a*) β_1 and (*b*) β_2 (see text). Estimated values of b_∞ are indicated on the b_L axis.

which also yields the equilibrium droplet shape (see Zia and Avron 1982 for details and references). $R(\hat{r})$ is the radius vector from the centre of symmetry of the droplet to the surface in direction $\hat{r}$ and $\sigma(\hat{n})$ is the free energy per unit area of an interface normal to $\hat{n}$. (8) and (9) are valid for arbitrary lattices and dimensionalities, while in the special case of the square lattice the exactly known form for $\sigma(\hat{n})$ (Rottmann and Wortis 1981, Avron *et al* 1982) leads to the following explicit equation for the Wulff construction (Zia and Avron 1982):

$$\cosh(\beta x) + \cosh(\beta y) = \cosh^2(2\beta J)/\sinh(2\beta J) \tag{10}$$

(10) is actually a special case of a more general result for anisotropic couplings. At $T = 0$ the droplet profile described by (10) is a square: for any $0 < T < T_c$ the flat sides of the square are rounded out, a feature connected with the lack of a roughening transition in 2D (for a review see Rottmann and Wortis 1983). The droplet profile becomes more and more circular as T approaches T_c, consistent with the expected isotropy at the scaling limit.

Using symmetry considerations we can write down the following Fourier expansion for $r^2(\phi) = x^2 + y^2$ in terms of the polar angle ϕ:

$$r^2(\phi) = A_0 + \sum_{n=1}^{\infty} A_n \cos 4n\phi \tag{11}$$

then

$$W = 2\int_0^{\pi/4} r^2(\phi)\,\mathrm{d}\phi = \pi A_0. \tag{12}$$

Approximate hand calculations for W at temperatures β_1 and β_2 were carried out by truncating (11) at the third term and fitting it to (10) for $\phi = 0$, $\tan^{-1}(\frac{1}{2})$ and $\frac{1}{4}\pi$. W was obtained from the resulting value of A_0 using (12). The results, accurate to the four significant figures quoted, are

$$\begin{aligned} \beta = \beta_1: &\qquad W = 10.38\beta^{-2} \\ \beta = \beta_2: &\qquad W = (3.366\times 10^{-2})\beta^{-2}. \end{aligned} \tag{13}$$

Substitution of (13) into (8), (7*a*) yields the figures for $1/2A$ shown in the second row of table 1. We have used the exact (Yang 1952) result for the magnetisation: $M = (1-\mathrm{cosech}^4\, 2\beta J)^{1/8}$. Agreement with the corresponding b_∞ estimates is excellent, thus lending considerable support to the critical droplet idea which leads to the form (1).

Table 1. Comparison of b_∞ estimates of figure 1 with droplet model $1/2A$. Figures in brackets denote errors in last digit(s).

	$\beta = \beta_1$: $\exp -4\beta_1 J = 0.1 \exp -4\beta_c J$	$\beta = \beta_2$: $\exp -4\beta_2 J = 0.9 \exp -4\beta_c J$
b_∞	0.963(3)	24.95(10)
$1/2A$	0.964	25.0

We make the following three points. First, the order of magnitude difference in the values of b_∞ at the two temperatures is entirely due to a corresponding behaviour in the surface free energy, secondly the anisotropy in the surface tension at the lower temperature must be taken into account in order to yield the observed agreement while lastly, at the higher temperature, the renormalisation of the droplet volume term in (4) is important—without it the calculated value of $1/2A$ would be increased by 20%.

Our final calculation will be to obtain an expression for $1/2A$ as $T \to T_c$. Using (7*a*), (8), (10), (12) and the exact M, we have

$$\begin{aligned} 1/2A &= \pi^{-1}2^{-27/16}\{\ln(\sqrt{2}+1)\}^{-15/8}t^{-15/8} \\ &= 0.1251t^{-15/8}. \end{aligned} \tag{14}$$

Here t = reduced temperature $(T_c - T)/T_c$. The exponent in (14) is a universal quantity which could have been obtained by applying the usual scaling arguments to (1). The non-universal prefactor is in remarkable agreement with the estimate $0.124 + 0.01$ from the series analysis work of BK.

We conclude with some comments on possible generalisations of the present work. The Ising model on a square lattice is the only case for which an analytic expression for the surface free energy is available for all T right up to T_c and in any direct extension of the present work to other lattices this quantity would have to be evaluated approximately using the solid-on-solid model or Monte Carlo methods. The former approach is exact at $T = 0$ and is expected to yield good results at low temperatures (see Rottmann and Wortis (1983) for a review and reference list) while the latter

gives reasonable results for the surface energy and hence for Σ by integration, up to T_c. (Binder and Kalos 1980—see also Jacucci *et al* 1983). Three dimensional lattices are of particular interest because of the existence of a roughening transition at a finite temperature, below which the fluctuations of the critical droplet will be constrained by the presence of facets, thus modifying the exponent b from the value in (1c). Another feature of the Ising model in three dimensions, however, is the percolation of the minority phase at a temperature T_p below T_c (Muller–Krumbhaar 1974). This leads to the expectation that the expression for A in (7a), which is based on a non-interacting cluster picture of the minority phase, will only be valid at temperatures well below T_p. Unfortunately the presently available series for $M(H)$ in three dimensions are far too short (~six terms) to make any sensible comparison with the droplet theories.

In contrast, there is a wealth of series and Monte Carlo data for the 2D percolation problem, in which the cluster numbers above p_c have been fitted to the following asymptotic form (for a review see Stauffer 1979)

$$C(n) \sim \exp(-Dn^{1/2}). \tag{15}$$

The well known connection between bond percolation and the $s \to 1$ limit of the s-state Potts model has been exploited by Lubensky and McKane (1980)—see also Harris and Lubensky (1981)—to show that the form (16) is a consequence of the singularity structure (1) for the s-state Potts model (where H is now a field coupling to one of the s states). A primitive droplet theory yields a simple expression, analogous to (7a), for D in terms of the one-state limit of the surface free energy $\Sigma(s)$ of an equilibrium droplet in the Potts model. It would be interesting to investigate whether $\Sigma(1)$ has a simple interpretation in the percolation problem, and to obtain numerical values, perhaps by using an analytic continuation of a solid-on-solid method, in order to make a comparison with the existing data for D.

Finally, we remark that the determination of the non-universal prefactor B in (1a) is a much more difficult problem, requiring a lattice treatment of the droplet wobble fluctuations.

I wish to thank Professor D J Wallace for suggesting this problem and for stimulating discussions.

Note added in proof. The present droplet theory has been extended to treat the Hamiltonian field theory version of the Ising model in (1+1)D (Harris 1984). We find very good numerical agreement with the results of a recent finite-lattice study. Reference, Harris C K 1984 *J. Phys. A: Math. Gen.* (to be submitted).

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