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LETTER TO THE EDITOR

Instantons and the Ising model below T_c

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Abstract. Recent series expansion estimates of the lattice Ising model suggest strongly that at fixed temperature below T_c the perturbation expansion of the magnetisation as a power series in the external field is asymptotic. We show that the published results are in excellent agreement with the universal features of the essential singularity predicted by field theory calculations using instantons and discuss further tests of the latter.

In an important paper Langer (1967) discusses the nature of the singularity at a first-order phase transition, in the contexts of a simple droplet model (for review and further references see Fisher (1967), Binder (1976)) and a ϕ^4 field theory. Denoting by H the external field which stabilises one phase or the other according as $H<0$ or $H>0$, the free energy/unit volume, F, of the droplet model of the phase which is stable for $H>0$ is shown to have a cut along the negative H axis when analytically continued in H. The discontinuity across the cut, or equivalently the imaginary part of F, arises from the existence of a critical droplet of radius $R_c \propto 1/|H|$, at a local *maximum* of the energy, where the steepest-descent evaluation of the integral over droplets of all radii moves into the complex R plane. In the ϕ^4 model with reduced Hamiltonian

$$\mathscr{H} = \int d^d x[\tfrac{1}{2}(\nabla\phi)^2 - \tfrac{1}{2}\mu^2\phi^2 + \tfrac{1}{4}g\phi^4 - H\phi], \qquad (1)$$

there is a real free energy defined by the functional average over the field $\phi(x)$ with $\langle\phi\rangle>0$ for $H>0$. The continuation of this free energy to $H<0$ cannot yet be done in a controlled fashion, but Langer showed that there is an extremum of $\mathscr{H}$ for a solution ϕ_c of the classical field equations $\nabla^2\phi = -\mu^2\phi + g\phi^3 - H$, which corresponds to a critical droplet in the above sense; $\phi_c(x)$ is radially symmetric and changes smoothly, over a distance μ^{-1}, between the two minima $\phi_\pm \simeq \pm\mu/\sqrt{g}$ at a radius $R \simeq \mu^2/(H\sqrt{g})$. The instability of this droplet solution to changes in its radius is interpreted by analogy with the simple droplet model, as giving rise to an imaginary part of F, through the steepest descent into the complex plane of the corresponding integration variable.

It was later recognised that the same technique could be used to describe the decay of a metastable state in a quantum field theory (Voloshin *et al* 1975, Coleman 1977, Callan and Coleman 1977, Stone 1977, Katz 1978, Affleck 1979). The field configuration which dominates the tunnelling process is, in the semiclassical limit, a solution of the classical field equations in imaginary time, i.e. precisely as above but with an extra spatial dimension for the imaginary time. The 'instantons' of the title refers to these

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classical solutions and continues the usage of the word in (thermal or quantum) tunnelling processes.

With the exception of Affleck (1979), none of these papers pushes the calculation of the determinant of the fluctuations as far as Langer's original paper. Generalisation of Langer's work to d dimensions is described in Wallace (1978) and Günther *et al* (1980). The result of these calculations for the imaginary part of F continued from $H>0$ to $H<0$ is

$$\operatorname{Im} F(H; \arg H = \pi) = -B|H|^b \exp -\{A|H|^{-a}[1+\mathrm{O}(H^2)]\}. \tag{2a}$$

We have shown explicitly only the H dependence, in the limit $H \to 0$. The quantities A and B depend upon temperature and the particular model (ϕ^4 or other) and are not universal. In the exponential factor, the power a is universal:

$$a = d-1. \tag{2b}$$

This exponential factor comes directly from the classical calculation ($\exp -\mathscr{H}(\phi_c)$). The power b in the prefactor is also universal:

$$b = \begin{cases} (3-d)d/2, & 1<d<5, d \neq 3 \\ -\frac{7}{3}, & d=3. \end{cases} \tag{2c}$$

As described in Langer (1967) and Günther *et al* (1980) there are two basic sources of this power b in the calculation of the fluctuation determinant: (i) the zero modes of the translation invariance broken by $\phi_c(x)$ must be handled by a transformation to collective coordinates and the resulting Jacobian factor gives a contribution to b; (ii) in the limit $H \to 0^-$ the radius of the critical droplet goes to infinity and the fluctuations representing the soft wobbles of the droplet away from the spherical give another singular factor. (The result (2c) corrects an error in Langer's paper ($d=3$) and differs from equation (24) in Wallace (1978) because the latter does not incorporate the second effects above.) As regards signs, A is of course a positive quantity; the simple droplet model provides a reliable guide to the overall sign of Im F such that, as written in (2a), B is also positive.

It should be stressed that equation (2) is the result of a semiclassical calculation; no explicit calculation of fluctuations with two or more loops has been made. This is potentially very serious because in the limit of interest ($H \to 0^-$), the soft wobbles of the droplet surface correspond to a gapless Goldstone mode which could, through infrared singularities in loop integrals, wreak havoc with the prediction (2). The results of the paper of Günther *et al* (1980) can be summarised as indicating that the form (2) should be (a) valid beyond the semiclassical limit and (b) universal.

We contend therefore that (2) correctly represents the singularity at the tip of this cut in the H plane. Our aim is to show that this singularity agrees with the numerical results of Baker and Kim (1980), denoted hereafter by BK. Using the low-temperature series expansions of Baxter and Enting (1979), and Sykes *et al* (1973, 1975) for the Ising model on various lattices, BK consider the magnetisation $M(T, H)$ as a power series in the reduced external field H at fixed temperature $T<T_c$. The coefficients in the expansion of $\bar{M} \equiv (1-M)/2$ in powers of H in the form

$$\bar{M} \sim \sum_{L=0} \bar{M}_L(-2H)^L \tag{3a}$$

are reproduced in table 1 for the particular case of the square lattice and at a temperature $\exp(-4\beta J) = 0{\cdot}1 \exp(-4\beta_c J)$. The ratios of these coefficients are plotted

Table 1. The estimated values $\bar{M}_L$ (equation (3a)) for the square lattice taken from Baker and Kim (1980). Also shown are coefficients b_L and c_L (equations (8a) and (9)). The uncertainties in the last digits are at most ±1, unless as shown in brackets.

L	$\bar{M}_L$	b_L	c_L
1	$0{\cdot}340\,676\times10^{-3}$		
2	$0{\cdot}198\,419\times10^{-3}$	0·291 214 (2)	
3	$0{\cdot}895\,862\times10^{-4}$	0·150 500	
4	$0{\cdot}392\,154\times10^{-4}$	0·109 435	
5	$0{\cdot}194\,603\times10^{-4}$	0·099 248	
6	$0{\cdot}115\,696\times10^{-4}$	0·099 087	
7	$0{\cdot}807\,868\times10^{-5}$	0·099 753	
8	$0{\cdot}641\,871\times10^{-5}$	0·099 3156 (2)	
9	$0{\cdot}569\,247\times10^{-5}$	0·098 5395 (3)	0·237
10	$0{\cdot}557\,617\times10^{-5}$	0·097 9570 (3)	0·248
11	$0{\cdot}598\,638\times10^{-5}$	0·097 5968 (3)	0·208
12	$0{\cdot}699\,371\times10^{-5}$	0·097 3559 (3)	0·183
13	$0{\cdot}883\,482\times10^{-5}$	0·097 1733 (2)	0·178
14	$0{\cdot}120\,013\times10^{-4}$	0·097 0292 (8)	0·177
15	$0{\cdot}174\,467\times10^{-4}$	0·096 9156 (12)	0·173 (3)
16	$0{\cdot}270\,29\times10^{-4}$	0·096 827 (4)	0·16 (1)
17	$0{\cdot}444\,58\times10^{-4}$	0·096 754 (6)	0·16 (2)
18	$0{\cdot}773\,81\,(2)\times10^{-4}$	0·096 697 (5)	0·15 (3)
19	$0{\cdot}142\,09\,(2)\times10^{-3}$	0·096 64 (2)	0·2 (1)
20	$0{\cdot}274\,54\,(5)\times10^{-3}$	0·096 60 (3)	
21	$0{\cdot}556\,8\,(2)\times10^{-3}$	0·096 58 (5)	
22	$0{\cdot}118\,29\,(4)\times10^{-2}$	0·096 57 (6)	
23	$0{\cdot}262\,7\,(4)\times10^{-2}$	0·096 6 (2)	
24	$0{\cdot}609\,(2)\times10^{-2}$	0·096 6 (4)	

in BK against L and there is a clear linear increase with L. BK quote for large L

$$\bar{M}_L/\bar{M}_{L-1}=C(L+L_0) \tag{3b}$$

with $L_0=0{\cdot}1\pm0{\cdot}2$. They conclude that the power series expansion in H has zero radius of convergence and $H=0$ is a singular point for $T<T_c$.

In order to compare expressions (2) and (3), we follow Günther *et al* (1980) by using the Cauchy integral formula with the contour enveloping the cut:

$$F(H)=\frac{1}{\pi}\int_{-\infty}^{0}\frac{\operatorname{Im}F(\arg H'=\pi)}{H'-H}\,\mathrm{d}H', \tag{4}$$

discarding the contour at infinity. (The argument is not affected if a finite number of subtractions is required.) Formally expanding in H, following the convention in equation (3a), we obtain

$$F(H)\sim\sum_{L=0}F_L(-2H)^L$$

where

$$F_L=\frac{1}{\pi(-2)^L}\int_{-\infty}^{0}\mathrm{d}H'(H')^{-(L+1)}\operatorname{Im}F(\arg H'=\pi). \tag{5}$$

Substituting ($2a$) into (5) gives

$$F_L=\frac{BA^{b/a}}{\pi a}2^{-L}A^{-L/a}\Gamma\left(\frac{L-b}{a}\right)[1+\mathrm{O}(L^{(a-2)/a})]. \tag{6}$$

The corrections of order $L^{(a-2)/a}$ come from the order H^2 in ($2a$)—they are asymptotically negligible according to ($2b$) only in two and three dimensions ($a=2$ gives only a change in the unknown quantity B). (For a review of this and other approaches to high-order estimates see e.g. Wallace (1978), Zinn–Justin (1979).) Derivatives of (6) give the growth of other quantities of interest, e.g. $M=\partial F/\partial H$ implies

$$\bar{M}_L=(L+1)F_{L+1} \qquad (L>0)$$
$$=\frac{BA^{b/a}}{\pi a}2^{-(L+1)}A^{-(L+1)/a}(L+1)\Gamma\left(\frac{L-b+1}{a}\right)[1+\mathrm{O}(L^{(a-2)/a})]. \tag{7}$$

Note (i) that the connection between imaginary part and asymptotic behaviour is erroneously stated in BK and (ii) the simple droplet model is indeed a reliable guide to the signs of the coefficients ($B>0$).

In comparing (7) with the results from the Ising model in table 1, since A and B are non-universal and unknown *a priori*, we follow BK and take ratios of successive coefficients which should grow, according to (7), as $L^{1/a}$, with the unknown corrections now of order $L^{-2/a}$, because of cancellation. For $d=2$ ($a=b=1$), we plot in table 1

$$b_L\equiv\bar{M}_L/(L\bar{M}_{L-1}), \tag{8a}$$

which should behave according to (7) as

$$b_L=(1/2A)[1+(1-b)L^{-1}+\mathrm{O}(L^{-2})]. \tag{8b}$$

The coefficient L_0 of ($3b$) is predicted to be zero because $b=1$ in $d=2$. The $\mathrm{O}(L^{-2})$ correction can also be seen in the numerical results. We show in table 1 the coefficients

$$c_L\equiv-(b_L-b_{L-1})L^2(L-1)^2/(2L-1) \tag{9}$$

which should tend to the constant coefficient of $1/L^2$ in b_L as $L\to\infty$; they also seem to stabilise well for $L>10$. The numerical results thus seem to agree remarkably well with the structure (2) in two dimensions.

Corresponding tests of (2) can be made for other lattices in two dimensions, in other dimensions and for other thermodynamic quantities. For example, for $d=3$, the expansion in even powers of H in equation (2) predicts

$$\bar{M}_L/(L^{1/2}\bar{M}_{L-1})=(8A)^{-1/2}[1+\tfrac{23}{12}L^{-1}+\mathrm{O}(L^{-2})] \qquad (d=3). \tag{10}$$

As remarked in Günther *et al* (1980), the coefficient of the $\mathrm{O}(L^{-1})$ term may be correct only above a roughening temperature, below which the soft wobble effects may be absent. (A different temperature-dependent phenomenon is also claimed in Domb (1976).)

For $d\geqslant 4$, the corrections of order H^2 in ($2a$) are not negligible since $2-\alpha<0$, and must be retained explicitly in the integral (5), which can then be evaluated for large L by steepest descents. The result is

$$\bar{M}_L/(L^{1/3}\bar{M}_{L-1})=\tfrac{1}{2}(3A)^{-1/3}[1-DL^{-2/3}+\tfrac{4}{3}L^{-1}+\mathrm{O}(L^{-4/3})] \tag{11}$$

where D is non-universal, depending on the relative coefficients of H^{-3} and H^{-1} in the exponential in ($2a$).

Further tests are possible if the series expansions can be used to give reliable coefficients in the critical region, particularly in three or four dimensions. Explicit expressions for universal amplitudes for coefficients of H^L for low L can be obtained from the scaling Ising equation of state, which is known to order ϵ^3 (Wallace and Zia 1974) in $4-\epsilon$ dimensions; scaling behaviour for high L can be estimated from the form (2) improved by the renormalisation group equation for the free energy as in Brézin *et al* (1976) or (Houghton and Lubensky 1980) as in Rudnick and Nelson (1976).

It is inappropriate to end on remarks concerning behaviour in the critical region. The important feature of this paper is the rather strong evidence it presents for universal features of the essential singularity at a first-order phase transition. It will be instructive to determine the extent of this apparent universality.

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