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# Metastable states near the phase boundary: a finite-lattice study

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**Abstract.** The energy of the metastable vacuum in a complex magnetic field has been computed for the Hamiltonian field theory version of the Ising model in (1+1)D, using finite-lattice methods. Evidence is found for an essential singularity at the phase boundary, as predicted by the droplet model.

## 1. Introduction

The analytic structure of the free energy along a phase boundary has been a subject of intermittent discussion for many years (for reviews, see Binder 1976, Domb 1976). Here we shall only be concerned with the 2D Ising model, which has a first-order phase transition line at magnetic field $h=0$, temperature $T<T_c$. The question then concerns the structure of the free energy in the 'spin-up' phase, say, as one continues from $h>0$, where the spin-up state is stable, to $h<0$, where it is metastable.

The presently accepted view (Fisher 1967, Andreev 1964, Langer 1967) is that the metastable state decays by the formation and growth of clusters or 'droplets' of overturned spins. Correspondingly, its free energy acquires an imaginary part, and a cut in the complex $h$ plane, with branch point at $h=0$. The droplet model predicts that this branch point is an essential singularity, with a discontinuity across the cut of the form (Günther *et al* 1980)

$$\operatorname{Im} F(h+\mathrm{i}\varepsilon) = -B|h| \exp(-A/|h|), \qquad h<0. \tag{1}$$

Now a singularity of this form is very hard to detect by standard numerical methods. The exponentially small term (1) is 'non-perturbative' in character, and is not seen at all in conventional low-field series expansions. Thus the early investigations reached various and conflicting conclusions regarding the existence and nature of any branch cut (Domb 1976, Binder 1976).

More recent series work has generally supported the droplet model picture. Enting and Baxter (1980) performed high-field series expansions at two temperatures below the critical point, and concluded that the behaviour of their coefficients was consistent

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with the predicted essential singularity. Baker and Kim (1980) have approached the problem more indirectly. Using as raw data the low-temperature low-field series expansion coefficients of Baxter and Enting (1979), they constructed low-field series expansions for the magnetisation at fixed, finite temperature. The asymptotic behaviour of these coefficients at large order appeared to be linearly divergent. This demonstrates a zero radius of convergence for the series, and an essential singularity of the predicted type. These results have been further analysed by Lowe and Wallace (1980).

Finite-lattice techniques offer the means of investigating this problem more directly. In the present paper we study the Hamiltonian field theory version of the Ising model in (1+1)D (Fradkin and Susskind 1978). The field theory equivalent of free energy is the ground-state energy. Using finite-size scaling techniques (Hamer and Barber 1981a, b), we set out to compute the energy of the metastable ground state, or 'false vacuum', for complex values of $h$. Then we may test directly for the existence of the predicted discontinuity.

The results of the investigation may be briefly summarised. The finite-lattice eigenvalues were found to converge in a rather irregular fashion for complex $h$. This unfortunately precludes the use of sequence extrapolation techniques (Hamer and Barber 1981b, Hamer 1981), and so the finite-lattice method loses much of its power. Nevertheless, evidence of a discontinuity was found, and estimates of its magnitude were made by an extrapolation technique. They are in good agreement with the predicted form, equation (1).

The layout of the paper is as follows. In § 2, the problem is formulated in the field theory framework, and the method of calculation is briefly outlined. In § 3 the results are presented, while § 4 contains some discussion.

## 2. Formalism

The field theory Hamiltonian of the Ising model in (1+1)D is (Fradkin and Susskind 1978)

$$H = \sum_{m=1}^{M} [(1-\sigma_3(m)\sigma_3(m+1)) - x\sigma_1(m) - h\sigma_3(m)]. \tag{2}$$

Here the index $m$ labels sites on a spatial lattice, while the time variable is taken to be continuous. The $\sigma_i$ are Pauli matrices acting on a two-state spin variable at each site. Equation (2) is a low-temperature representation in which the coupling $x$ plays the role of a temperature variable, and $h$ is the magnetic field. The total number of sites is $M$, and periodic boundary conditions are assumed. The critical point lies at $x = x_c = 1$.

The field theory equivalent of the free energy is the ground-state energy, $E_0$, of the Hamiltonian (2). Below the critical coupling, we know that there are in fact two 'ground states' which are degenerate at $h = 0$, one with predominantly spins up ($\sigma_3 = +1$), and the other with predominantly spins down ($\sigma_3 = -1$). Let us denote their energies by $E_0^+$ and $E_0^-$ respectively.

These quantities obey certain symmetry relationships in the complex $h$ plane. First of all, they are real analytic:

$$E_0^{\pm}(h) = [E_0^{\pm}(h^*)]^*. \tag{3}$$

Secondly, since the Hamiltonian is symmetric under the transformation

$$\left.\begin{aligned} &h \to -h \\ &\sigma_3(m) \to -\sigma_3(m), \text{ all } m \end{aligned}\right\}, \tag{4}$$

then it follows that

$$E_0^{\pm}(h) = E_0^{\mp}(-h). \tag{5}$$

These relationships imply that the analytic continuations of $E_0^+$ and $E_0^-$ to the entire $h$ plane may be related to their values in the first quadrant (i.e. $h_R \geqslant 0$, $h_I \geqslant 0$ where $h_R$, $h_I$ are the real and imaginary parts, respectively, of the magnetic field).

Our object, then, is to calculate $E_0^+$ for negative $h_R$, where the spin-up state is the metastable or 'false vacuum' state, and to check whether it has a discontinuity across the negative $h$ axis of the form (1).

To this end, calculations have been made of the eigenvalues of the Hamiltonian (2) on a sequence of finite lattices up to size $M = 9$. The generation of the low-temperature basis states, and of the matrix elements of $H$ connecting them, was carried out by standard methods (Hamer and Barber 1981a). To find the eigenvalues of the resulting matrix, double precision subroutines from the EISPACK library were used. Unfortunately, it is impossible to use iterative procedures (such as the Lanczos method or the conjugate gradient method) to calculate the low-lying eigenvalues when $h$ is complex, and $H$ is non-Hermitian. This restricts the size of the matrices, and consequently the lattice sizes $M$, which can be dealt with.

## 3. Results

The first order of business is to identify the metastable 'false vacuum' state. For this purpose, the average magnetisation $\langle\sigma_3\rangle$ was computed for each state; and some typical plots of energy versus magnetisation are shown in figure 1. For small $|h_R|$, the plots have the classic 'double well' shape (figure 1(*a*)), and the false vacuum may be easily identified. As a working criterion, it was found satisfactory to define the two vacua as those states with $|\langle\sigma_3\rangle| > \frac{1}{2}$, whose energies had minimum real part.

For larger $|h_R|$, the second well disappears (figure 1(*b*)), and there is no longer any identifiable false vacuum. By making plots such as figure 1, one may estimate roughly the position of the stability limit for the metastable state; the results are shown in figure 2. Note that the two fixed points of this curve are at the critical point $x = 1$, $h_R = 0$, where the distinction between the two phases disappears, and at $x = 0$, $|h_R| = 2$, where the magnetic field term is just strong enough to counterbalance the pairing term in the Hamiltonian (2) for a single overturned spin. We have not explored the detailed shape of the limiting curve near the critical point.

We may now study the energy of the metastable state as a function of complex magnetic field $h$. It is convenient to subtract out the leading-order effect of the magnetic field, and to define a reduced energy per site

$$E_0^{+'} = E_0^+/M + h \tag{6}$$

for each lattice size $M$. Figure 3 shows a typical graph of $\mathrm{Im}(E_0^{+'})$ as a function of $h_I$ at fixed negative $h_R$, for various lattice sizes $M$. It can be seen that the finite-lattice eigenvalues converge to the bulk limit ($M \to \infty$) in a rapid but rather irregular fashion

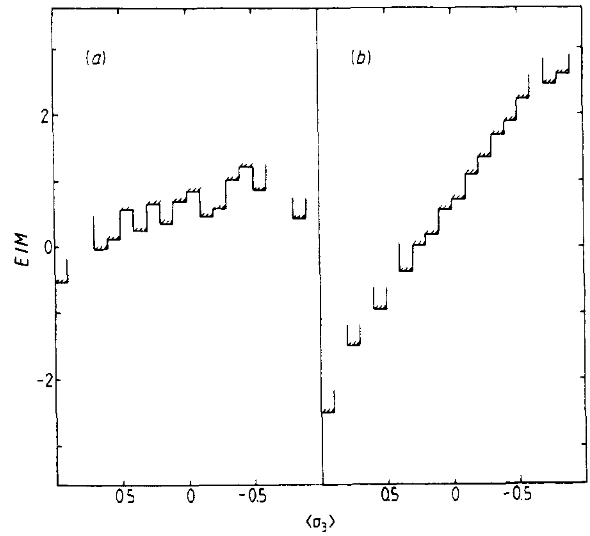


**Figure 1.** Plot of energy $E/M$ versus magnetisation $\langle\sigma_3\rangle$, at fixed coupling $x=0.4$, for lattice size $M=9$. ($a$) is at (real) magnetic field $h=-0.5$; ($b$) is at $h=-2.5$. The figure shows the minimum energy state in each magnetisation bin (not all bins are occupied).

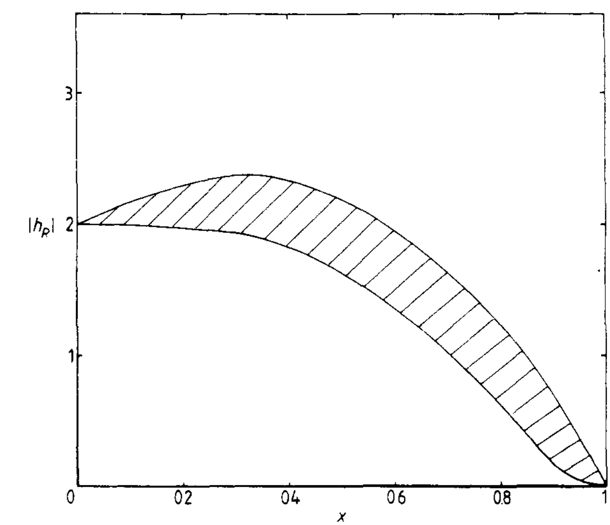


**Figure 2.** The stability limit for the metastable state as a function of (real) magnetic field $h_R$ and coupling $x$. The boundary is crudely estimated as lying somewhere in the shaded area, based on the results for $M=9$.

at fixed values of $h_I$. This irregularity appears to be associated with the occurrence of branch points in the eigenvalues in the complex $h$ plane. Unfortunately, it precludes the use of finite-size scaling sequence extrapolation methods (Hamer and Barber 1981b, Hamer 1981) to estimate the bulk limit, and so much of the power of the finite-lattice method is lost. Nevertheless, the raw finite-lattice sequence converges rapidly enough to allow an accurate estimate of the bulk limit at large values of $h_I$, as illustrated by the full lines in figure 3.

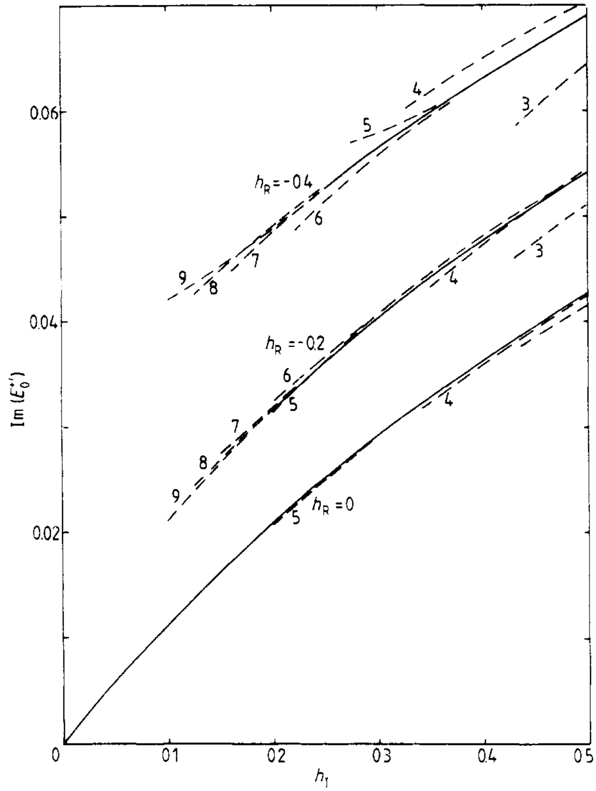


**Figure 3.** The imaginary part of the metastable vacuum energy per site, $\text{Im}(E_0^{+'})$, as a function of $h_I$, for three different values of $h_R$. The broken lines are finite-lattice results, labelled by the lattice size $M$. The full lines represent the 'bulk limit' (as defined in § 3), where it can be estimated to an accuracy within the width of the line. All results are at fixed coupling $x = 0.8$.

At small values of $h_I$, the finite-lattice sequence becomes much less rapidly convergent, and the bulk limit cannot be estimated directly with any confidence. This provides *a priori* evidence of a singularity in the neighbourhood. Our object now is to estimate the quantity

$$\Delta = \lim_{h_I \to 0} \text{Im}(E_0^{+'}). \tag{7}$$

A non-zero value of $\Delta$ corresponds to a discontinuity in the imaginary part, by the real analyticity property (3). Since finite-lattice sequence extrapolation methods (Hamer 1981) are useless in this case, the only method open to us is to perform an analytic continuation from the bulk limit estimated at larger $h_I$.

Our procedure for doing this runs as follows. First, the bulk limit is taken equal to the metastable eigenvalue for $M = 9$ (the largest lattice size available) for values of $h_I$ above some cut-off where sufficient convergence has been obtained. Next, this limiting curve is fitted with linear and quadratic forms at various values of $h_I$ above the cut-off†, and those forms are extrapolated to the axis $h_I = 0$. Some typical results

† For instance, the linear form used is simply the tangent to the bulk limit.

for the extrapolated values are depicted in figure 4. From these one may form an estimate of $\Delta$, as illustrated in figure 4; the discrepancy between the linear and quadratic extrapolants provides some idea of the likely error.

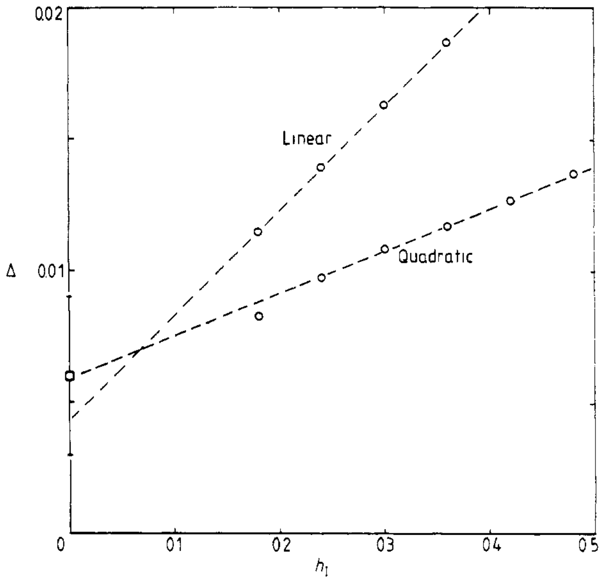


**Figure 4.** Linear and quadratic extrapolants for the value of $\Delta$, as a function of the point $h_I$ at which the series fits were made (see § 3). The broken lines are straight-line fits; the marked square is the final estimate of $\Delta$. All results are at a fixed value of the coupling $x = 0.8$, and $h_R = -0.2$. A cut-off has been applied at $h_I = 0.18$.

This procedure is open to serious question. After all, the $M = 9$ eigenvalue is a function, usually analytic†, which fits the 'bulk limit' (as defined above) exactly; yet its imaginary part at $h_I$ is always zero, since $H$ is a finite, Hermitian matrix in that case. It is only on the assumption that the bulk limit is relatively smooth, and shows no great increase in curvature near the real axis, that one can place any great reliance on our estimates. This assumption is reasonable provided one is well away from any second-order critical point. In any case, there seems to be no alternative method available in the circumstances.

The resulting estimates of $\Delta$ are listed in table 1. Two points are worth noting. First is the occurrence of estimates for $x = 1$, which should be excluded according to the stability limit of figure 2. This is possible because the stability limit recedes at finite values of $h_I$, allowing the procedure outlined above to be carried out even as $x \to 1$: the resulting estimates may be regarded as limiting cases. Secondly, no useful estimates were possible at small $x$ and large $h_R$: indeed, there was no real evidence of any finite discontinuity at all in that region, and we can only assume that the 'break' to discontinuous behaviour occurs at lattice sizes $M > 9$.

In figure 5 the estimates of $\Delta$ are plotted against $h_R$, for a particular coupling value $x = 0.8$. Also shown is a fit of the form predicted by Günther *et al* (1980), and Lowe

† Though not always: *vide* the branch points mentioned above.

**Table 1.** Estimates of $\Delta$ as a function of coupling $x$ and magnetic field $h_R$.

| $h_R$ \ $x$ | 0.2 | 0.4 | 0.5 | 0.6 | 0.8 | 1.0 |
|---|---|---|---|---|---|---|
| 0 | $(0\pm1)E-9$ | $(0\pm5)E-7$ | $(0\pm3)E-6$ | $(-4\pm5)E-5$ | $(-4\pm4)E-4$ | $(-1\pm4)E-3$ |
| 0.1 | $(0\pm1)E-9$ | $(0\pm1)E-6$ | $(0\pm1)E-5$ | $(0\pm4)E-5$ | $(0\pm4)E-3$ | $0.009\pm0.01$ |
| 0.2 | $(0\pm2)E-9$ | $(9\pm4)E-6$ | $(1\pm1)E-4$ | $(4\pm3)E-4$ | $0.006\pm0.003$ | $0.025\pm0.01$ |
| 0.3 | $(0\pm3)E-9$ | $(8\pm2)E-5$ | $(65\pm20)E-5$ | $(30\pm6)E-4$ | $0.020\pm0.003$ | $0.042\pm0.01$ |
| 0.4 | $(6\pm2)E-6$ | $(64\pm4)E-5$ | $(27\pm2)E-4$ | $(75\pm5)E-4$ | $0.031\pm0.005$ | $0.062\pm0.01$ |
| 0.5 | $(70\pm25)E-6$ | $(21\pm2)E-4$ | $(60\pm2)E-4$ | $0.013\pm0.001$ | $0.038\pm0.005$ | $0.082\pm0.007$ |
| 0.6 | — | — | $(6\pm2)E-3$ | $0.018\pm0.002$ | $0.056\pm0.005$ | $0.106\pm0.005$ |
| 0.8 | — | — | 0.017● 0.001 | $0.035\pm0.005$ | $0.08\pm0.01$ | |

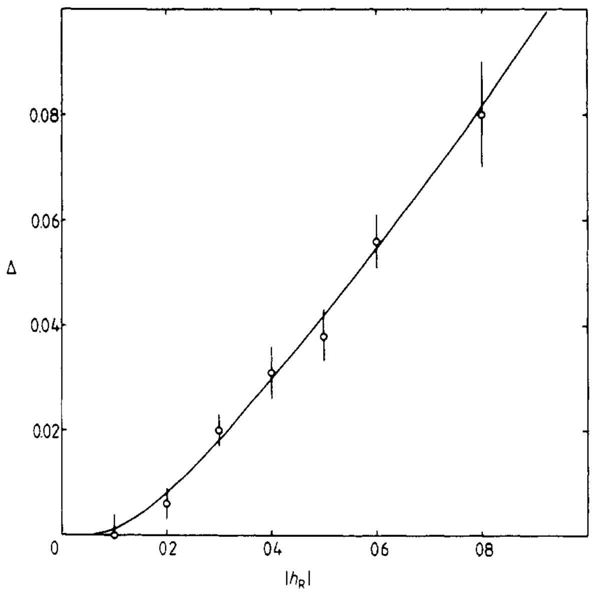


**Figure 5.** Graph of $\Delta$ against $|h_R|$ for $x=0.8$. The data points are our finite-lattice estimates, and the full line is a fit of the form (8), with $A=0.25$ and $B=0.14$.

and Wallace (1980):

$$\Delta = B|h_R|\exp(-A/|h_R|), \tag{8}$$

with $A=0.25$, $B=0.14$. It can be seen that the data are well fitted. In figure 6, the quantity $\log(\Delta/|h_R|)$ is plotted against $1/|h_R|$, for various values of $x$. The predicted form (8) corresponds to a straight line on this plot, and it is clear that straight lines fit the data quite well.

From these straight line fits, the parameters $A$ and $B$ may be estimated in each case, and the results are listed in table 2. The values of $B$ show little dependence on the 'temperature' variable $x$; while $A$ appears to diverge at low temperature, and to vanish as $x\to1$. This matches the sort of behaviour found by Baker and Kim (1980). The data are not sufficient, however, to test the critical behaviour of $A$ near $x=1$ (cf Baker and Kim).

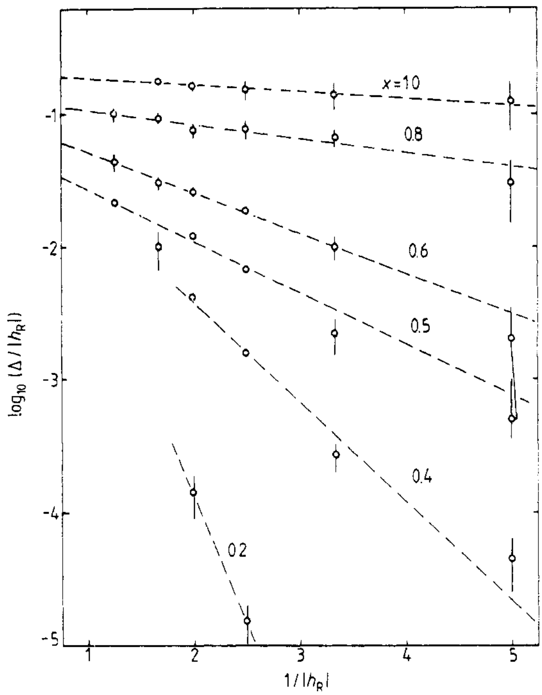


**Figure 6.** Graph of $\log_{10}(\Delta/|h_R|)$ against $1/|h_R|$ for various values of $x$. The data points are our finite-lattice estimates, and the broken curves are straight lines drawn through each set of data points.

**Table 2.** Estimates of the parameters $A$ and $B$, as a function of coupling $x$.

| $x$ | $A$ | $B$ |
|---|---|---|
| 0.2 | $4.4\pm1$ | $0.9\pm0.8$ |
| 0.4 | $1.7\pm0.2$ | $0.12\pm0.04$ |
| 0.5 | $0.89\pm0.1$ | $0.07\pm0.02$ |
| 0.6 | $0.70\pm0.1$ | $0.10\pm0.02$ |
| 0.8 | $0.25\pm0.1$ | $0.14\pm0.03$ |
| (1.0 | $0.13\pm0.1$ | $0.21\pm0.02$) |

## 4. Discussion

*A priori* evidence for a cut on the negative $h$ axis has been found in the slow convergence of the finite-lattice eigenvalues in that neighbourhood. The magnitude of the cut has been estimated by an extrapolation method from the results at complex $h$. It is in good agreement with the form for the essential singularity, equations (1) and (8), proposed by Günther *et al* (1980).

These results provide the first direct estimates, as far as we know, of the discontinuity $\Delta$. But since our extrapolation method is open to some doubt, as discussed in § 3, it would be useful to check the results for $A$ and $B$ against series estimates, similar to those of Baker and Kim (1980), in the field theory formulation. Conversely, it would be useful to compute finite-lattice estimates similar to ours in the Euclidean regime, using for instance the methods of Nightingale and Blöte (1980). An even more powerful technique might be to use variational methods such as those of Baxter and Tsang (1980).

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