INSTANTONS AND SURFACE TENSION AT A FIRST-ORDER TRANSITION

Sourendu Gupta
HLRZ, c/o KFA Jülich, D-5170 Jülich, Germany.

ABSTRACT

We study the dynamics of the first order phase transition in the two dimensional 15-state Potts model, both at and off equilibrium. We find that phase changes take place through nucleation in both cases, and finite volume effects are described well through an instanton computation. Thus a dynamical measurement of the surface tension is possible. We find that the order-disorder surface tension is compatible with perfect wetting. An accurate treatment of fluctuations about the instanton solution is seen to be of great importance.
First order phase transitions, i.e., phase coexistence points, have recently been subjected to intense analysis. Such systems are characterised by many different dimensionful quantities. It is useful to divide these into two classes of observables. The first pertains to properties of the pure phases. Such properties are obtained, as usual, by taking derivatives of the (extensive) free energy. These derivatives, or cumulants, are extracted through finite-size scaling. In recent years a full theory of such scaling has been developed [1,2] and tested [1–3]. The second class concerns coexistence. Foremost among such variables is the surface tension—the leading non-extensive part of the free energy. Most theories of the (canonical) dynamics at the phase transition involve the surface tension. The measurement of this quantity is usually approached through detailed investigations of the static system at the phase transition [4].

However, much of the recent attention enjoyed by first-order phase transitions is due to the interesting dynamics of the transition. This is expected to be due to nucleation. We perform a careful analysis of finite size effects in the equilibrium dynamics and compare our observations with an instanton-based computation [5]. We also test nucleation theory through a non-equilibrium process—hysteresis. Certain scaling laws for this have been proposed recently [6]; we verify them for the first time. These two tests provide the justification for the use of dynamical techniques for the measurement of the surface tension.

Our numerical work is done with a simple model—the two dimensional 15 state Potts model. This model is defined through the partition function and Hamiltonian

\[ Z = \sum_{\{\sigma_r\}} \exp(-\beta H), \quad H = \sum_{<rr'>} 1 - \delta_{\sigma_r,\sigma_{r'}}. \]  

(1)

where the spin \( \sigma_r \) sitting at the site \( r \) of a (square) lattice can take one of 15 values and the angular brackets denote nearest neighbours. At \( \beta_t = \log(\sqrt{15} + 1) \), ordered and disordered phases coexist in the thermodynamic limit. The two phases can be distinguished either through a singlet magnetisation or the internal energy density

\[ e = \frac{1}{L^2} \langle H \rangle, \]  

(2)

where the lattice size is \( L^2 \). In the thermodynamic limit, the internal energies in the ordered and disorder phases are, respectively, \( e_0 = 1.779 \) and \( e_d = 0.737 \).

Recent analysis of correlation lengths in Potts models [7] have yielded an exact result for a spin-spin correlation length. This has been identified with the correlation length in the disordered phase \( \xi_d \). A duality argument has been used [8] to relate the order-order surface tension, \( \sigma_{oo} \), to this correlation length—

\[ \sigma_{oo} = \frac{1}{\xi_d}. \]  

(3)
The perfect wetting conjecture would then imply the relation
\[ 2\sigma_{od} = \sigma_{oo} = \frac{1}{\xi_d}. \]  
(4)

between the order-disorder surface tension, \( \sigma_{od} \), and the rest of these quantities. Although proven only in the limit \( q \to \infty \), it is strongly suspected that perfect wetting holds for two dimensional Potts models for all \( q > 4 \). From the formulae of [7] one finds \( \xi_d = 4.18 \) for \( q = 15 \); implying \( 2\sigma_{od} = 0.239 \). Thus a quantitative test of nucleation theory should yield this value for \( \sigma_{od} \). Alternately, the argument can be turned around and the measurement of the single quantity, \( \sigma_{od} \), can be used to check the perfect wetting conjecture.

One of the dynamical methods we use is a finite-size scaling of the exponential autocorrelation time, \( \tau \), of the energy density. Through a study of the 10-state Potts model, numerical evidence was presented in [9] that this autocorrelation time is determined by the tunnelling rate between the coexisting ordered and disordered phases. As a result, the autocorrelation time can be identified with the outcome of an instanton computation [5] giving
\[ \tau^{-1}(L) = aL^{-d/2} \exp(-2\sigma_{od}L^{d-1}). \]  
(5)

In our case, of course, \( d = 2 \). The exponential factor is the saddle-point result; and the \( L \)-dependence of the prefactor is obtained from a one-loop computation of the determinant of the fluctuations around the saddle point. The test of the instanton computation is in the \( L \)-dependence of the measured values of \( \tau \). Note that Eq. (5) describes dynamics in equilibrium.

We also study a particular example of off-equilibrium dynamics, that of hysteresis. The coupling \( \beta \) is cyclically varied about the critical coupling \( \beta_t \) with a frequency \( \omega \) and an amplitude \( \Delta \beta \). Hysteresis occurs as \( \varepsilon \) switches between the values \( \varepsilon_o \) and \( \varepsilon_d \). The area of the hysteresis loop in the energy density, \( A(\omega) \) is studied as a function of \( \omega \). The system has a real-time excitation with a ‘mass’ given by Eq. (5). The measurement of \( A(\omega) \) is really a ‘line-shape’ measurement. When \( \Delta \beta \to 0 \), the peak should be at \( \tau^{-1}(L) \) and the shape should be approximately Lorentzian. This cannot be converted to an useful test because the functional form of the finite \( \Delta \beta \) corrections is not known.

We define the coercive coupling \( \delta \beta_c \) through the fact that hysteresis loops reach the value \((\varepsilon_o + \varepsilon_d)/2\) when the coupling is \( \beta_t \pm \delta \beta_c \). Here the nucleation rate becomes larger than \( 1/\omega \), and the probability of a flip into the stable phase exceeds \( 1/2 \). This argument was presented in [6] and was developed into the scaling law
\[ A(\omega) \sim (\ln \omega)^{-1/(d-1)} \quad \text{where } \omega \to 0. \]  
(6)
The coercive coupling also obeys the same scaling law. Verification of this relation thus furnishes a test of nucleation theory. Furthermore, since the tunnelling rate is finite for any finite lattice, \( A(\omega) \) is zero at some non-zero frequency \( \Omega \), and we have the relation

\[
\Omega(L) = \tau^{-1}(L) \quad \text{where } A(\Omega) = 0.
\] (7)

Thus the scaling of \( \Omega \) with \( L \) is again given by Eq. (5), and constitutes yet another test of nucleation theory. Note that Eq. (6) refers to a slow non-equilibrium situation.

**TABLE 1.**

Run parameters for the two-dimensional 15-state Potts model. We show the lattice sizes \( L \), pseudo-critical couplings \( \beta_T(L) \), statistics used for the determination of autocorrelation times, \( N_{run} \), and the hysteresis parameters \( \beta_m, \Delta \beta \) and \( \delta \beta \).

| \( L \) | \( \beta_T(L) \) | \( N_{run} \) | set 1 | set 2 | set 3 |
|---|---|---|---|---|---|
| | | | \( \beta_m \) | \( \Delta \beta \) | \( \delta \beta \) | \( \beta_m \) | \( \Delta \beta \) | \( \delta \beta \) | \( \beta_m \) | \( \Delta \beta \) | \( \delta \beta \) |
| 8 | 1.546 | \( 1 \times 10^6 \) | 1.65 | 0.200 | 0.010 | 1.61 | 0.060 | 0.005 | 1.6470 | 0.1620 | 0.0135 |
| 12 | 1.5661 | \( 1 \times 10^6 \) | 1.65 | 0.100 | 0.005 | 1.61 | 0.060 | 0.005 | 1.6260 | 0.108 | 0.009 |
| 16 | 1.5723 | \( 2 \times 10^6 \) | 1.61 | 0.080 | 0.005 | 1.61 | 0.060 | 0.005 | 1.6470 | 0.1620 | 0.0135 |
| 20 | 1.5772 | \( 4 \times 10^6 \) | 1.61 | 0.060 | 0.005 | 1.61 | 0.060 | 0.005 | 1.6260 | 0.108 | 0.009 |
| 24 | 1.5798 | \( 5 \times 10^6 \) | 1.61 | 0.060 | 0.005 | 1.61 | 0.060 | 0.005 | 1.6260 | 0.108 | 0.009 |
| 30 | 1.5811 | \( 4 \times 10^7 \) | 1.61 | 0.060 | 0.005 | 1.61 | 0.060 | 0.005 | 1.6260 | 0.108 | 0.009 |

For Potts models at phase coexistence it was observed [9] that both local and Swendson-Wang dynamics are dominated by tunnellings, and that the exponential autocorrelation times, with changing \( \beta \) and \( L \), are related by a constant. In view of this, all our simulations were performed with the latter algorithm. Autocorrelation times were measured at the pseudo-critical couplings, \( \beta_T(L) \), defined by the maximum of the specific heat. For \( L \leq 20 \) the values of \( \beta_T(L) \) and \( \tau \) were obtained in [10]; this work verifies these measurements. Hysteresis was induced by cyclically changing \( \beta \) from a maximum of \( \beta_m \) down by an amount \( \Delta \beta \) and back, in discrete steps of \( \delta \beta \), running \( N \) sweeps of a Swendson-Wang update at each coupling. The runs were started by first thermalising a system at \( \beta_m \) with \( 2 \times 10^5 \) cluster updates. Then for each \( N \) (and fixed values of the other parameters) we ran through 200 hysteresis cycles. Since fairly large values of \( N \) had to be used, this was by far the most CPU-intensive part of these computations. The run parameters are shown in Table 1. Three different sets of parameters were used in order to check that the scaling law of Eq. (6) and the extrapolated values of \( \Omega(L) \) were independent of \( \Delta \beta \).
For each hysteresis loop, we defined the area by the sum
\[ A = \delta \beta \sum_i (-1)^D \bar{e}_i, \]  
(8)
where \( i \) labels each of the values of \( \beta \) in the cycle, the bar above \( e_i \) denotes averaging over the \( N \) sweeps performed at that \( \beta \). The value of \( D \) was set to be equal to 0 in that half of the cycle with decreasing \( \beta \), and 1 in the other. The averages and errors were obtained by jack-knife estimators over all the cycles.

A second measurement was of the cyclic response function
\[ c^i_V = \langle (e_i - \langle e_i \rangle)^2 \rangle, \]  
(9)
where the angular brackets denote averages over all measurements performed at a given coupling in the hysteresis cycle. This response function peaks twice during a cycle, at \( \pm \delta \beta_c \), and allows us to extract \( \delta \beta_c \) by searching for the maximum of \( c^i_V \). This procedure is the dynamical analogue of defining the transition coupling on a finite lattice, \( \beta_T(L) \) by the peak in usual response function \( c_V \).

The average and error were again estimated by a jack-knife procedure. These measurements of \( \delta \beta_c \) have larger relative errors than \( A \). This is due to two reasons. The first is intrinsic. Since tunnellings occur at random times, there is a cycle to cycle variation in the coupling at which tunnellings occur. The other error is related to the statistics. The identification of the coercive coupling depends on the relative heights of the two peaks, and is subject to fairly strong errors. Due to these uncertainties, we decided not to use this quantity for our scaling tests.

The frequency \( \omega \) should be identified with \( 2\pi \delta \beta /N \Delta \beta \). However, for each \( L \), since \( \delta \beta \) as well as \( \Delta \beta \) are fixed inside each set, these factors are not important when trying to check the scaling with \( \omega \). Furthermore, when comparing different values of \( L \), we are interested in time scales expressed directly in sweeps. Hence we shall use the convention \( \omega = 1/N \). This is only a matter of convenience. When necessary, one should use the full definition of \( \omega \).

For each \( L \) and a set of \( \omega \) at fixed \( \Delta \beta \) and \( \delta \beta \), we tried to fit the data on \( A(\omega, \Delta \beta) \) to a Lorentzian. We found that this description improves as \( \Delta \beta \) decreases. This is illustrated in Fig. 1 for the \( L = 16 \) lattice. At low frequencies, where the data deviates from the Lorentzian shape, \( A(\omega) \) is independent of \( \Delta \beta \). For large \( N \), when the data deviate from the Lorentzian shape, we fit a form
\[ A(\omega) = a - b/\log N. \]  
(10)
We found extremely good fits to this form and could certainly rule out any power-law behaviour. The data and fits are shown in Fig. 2. The fitted parameters \( a \) and \( b \) give
Hysteresis loop areas $A(\omega)$ as functions of $1/N$ for the 15-state Potts model on $16^2$ lattices. The data are for sets 1 (squares), 2 (circles) and 3 (triangles) of Table 1. The lines show the best Lorentzian fits.

estimates of $\Omega$— the frequency at which the loop area vanishes. Errors on $\Omega$ were estimated from the covariance matrix between these parameters. We found good agreement between these values obtained indirectly and the direct measurements of $\tau(L)$. The scaling of $\Omega^{-1}(L)$ with $L$ is consistent with Eq. (5), but does not provide a very stringent test. The direct measurements of $\tau(L)$ are, of course, more accurate.

The direct measurements of $\tau(L)$ were obtained by constructing the autocorrelation function and fitting its long-distance form to an exponential. As a cross check, we measured local masses and looked for plateaus as a signal that a single mass fit over a given range was reasonable. The measurement procedure remains the same as in [9]. In all cases the fits were performed over a range which turned out to be $\tau < t < 4\tau$. The errors on $\tau(L)$ were, of course, reflections of the errors on the autocorrelation function. These were obtained as the dispersion between jack-knife blocks. We varied the number of jack-knife blocks between 5 and 25. We took the lack of sensitivity of the means and errors to the number of blocks as an indication that our error estimates are reliable.

In order to test Eq. (5) and measure $\sigma_{od}$, we fitted the data on $\tau(L)$ to the form

$$\log(\tau/L) = cL + c'.$$

Note that $\sigma_{od}$ is given by $c/2$. On the left hand side of Eq. (11), the division by
Hysteresis loop areas $A(\omega)$ as functions of $1/\log N$ for the 15-state Potts model for $L = 8$ (filled circles), 12 (filled circles), 16 (filled squares) and 20 (open squares). The lines show the best fits.

$L$ takes care of the effects of fluctuations around the instanton solution. It turns out that this term in the fit is quite crucial. An attempt to perform the fit without this factor was completely unsuccessful; $\chi^2$ values obtained increased by almost an order of magnitude. In principle, one could perform a three-parameter fit, leaving the power of $L$ in the pre-exponential factor to be determined by the data. Unfortunately this requires more lattice sizes than we had in this study. Our fits gave

$$2\sigma_{od} = 0.263 \pm 0.009 \quad (\chi^2 = 1.0/2 \text{ dof}, \ 16 \leq L \leq 30).$$

This result is compatible with perfect wetting.

Although the difference between the perfect wetting result for $\sigma_{od}$ and our measurement is not statistically significant at the 3σ level, we believe it deserves comment. We find it difficult to regard seriously the possibility that perfect wetting begins to break down when $q$ drops to a number close to 15. More likely is that Eq. (5) has to be supplemented with a higher loop computation. It has been argued [5] that a loop-wise expansion of the pre-exponential factor yields a power series in $L^{-d/2}$. It is a reasonable guess that the two-loop term is marginally important for the lattice sizes we have worked with. Then our observations would imply that the coefficient of the term in $L^{-d}$ is positive. A computation of this term would certainly be useful.
We show the scaling of $1/\Omega$ (open circles) and directly measured values of the autocorrelation time at $\beta_r(L)$, $\tau$, (filled circles) against the lattice size $L$. The lines show the best fits of the form shown in Eq. (13). The values of $1/\Omega$ have been multiplied by 2 for visibility.

Finally we comment on previous numerical tests of Eqs. (5) and (6). A high-statistics study of the 10-state Potts model [9] had established that the autocorrelation time in equilibrium was determined by the tunnelling phenomenon. However, this study had not been able to observe even the dominant exponential behaviour in Eq. (5). It was conjectured there that $L/\xi$ values used there were too small. The recent work of [7,11] shows that this is indeed correct. In that study the largest values of $L$ used were about $3\xi$, whereas this study uses between $4\xi$ and $7\xi$.

Earlier studies of the scaling of $A(\omega)$ with $\omega$ had parametrised the variation by power laws. This is presumably correct for some systems, but the arguments of [6] must hold whenever the dominant dynamical mechanism is nucleation and tunnelling. Magnetic hysteresis in the Ising model, or the one-component $\phi^4$ theory should therefore be described by Eq. (6). The contradictory results of [12] were obtained with values of $\omega$ much smaller than the ones we use. The implication is that Eq. (6) is not applicable to these.

We summarise the main results obtained in this study. The scaling law of Eq. (6) for the frequency dependence of hysteresis loop areas is found to hold extremely well
over three decades in frequency, and for a variety of lattice sizes. This is strong evidence that in the particular non-equilibrium situation at a first-order phase transition exemplified by hysteresis, the dynamics is of nucleation. Furthermore, the expression in Eq. (5) is found to describe the finite-size scaling of the autocorrelation times, showing that an instanton based description of the equilibrium dynamics is valid. A proper treatment of fluctuations around the instanton is observed to be crucial for the description of the data. The dynamics then allows the extraction of the surface tension. For the 15-state Potts model we find that perfect wetting holds. A statistically insignificant discrepancy can be attributed to the neglect of two-loop terms in the treatment of the fluctuation determinant. It should be emphasised that this makes the present computation one of the most accurate measurements of a surface tension to date.
REFERENCES

1) C. Borgs and R. Kotecký, J. Stat. Phys. 61 (1990) 79;
   C. Borgs, R. Kotecký and S. Miracle-Solé, J. Stat. Phys. 62 (1991) 529;
   C. Borgs and W. Janke, Phys. Rev. Lett. 68 (1992) 1738.
2) S. Gupta, A. Irbäck and M. Olsson, preprint HLRZ 23/93 and LU-TP-93-6,
   Nucl. Phys. B, in press.
3) A. Billoire, R. Lacaze and A. Morel, Nucl. Phys. B370 (1992) 773;
   B. Berg, A. Billoire and T. Neuhaus, Saclay preprint SPhT-92/120.
4) K. Binder, Z. Phys. B 43 (1981) 119;
   K. Kajantie, L. Kärkkäinen and K. Rummukainen, Phys. Lett. B223 (1989) 213;
   J. Potvin and C. Rebbi, Phys. Rev. Lett. 62 (1989) 3062;
   K. Jansen et al., Nucl. Phys. B322 (1989) 693.
5) J. C. Niel and J. Zinn-Justin, Nucl. Phys. B280 [FS18] (1987) 355.
6) D. Dhar and P. B. Thomas, preprint TIFR/TH/92-32.
7) E. Buffenoir and S. Wallon, Saclay preprint, SPhT/92-077.
8) C. Borgs and W. Janke, preprint HLRZ 54/92 and FUB-HEP 13/92.
9) A. Billoire, R. Lacaze, A. Morel, S. Gupta, A. Irbačk and B. Petersson, Nucl.
   Phys. B358 (1991) 231.
10) M. Ohlsson, B. Sc. Thesis, University of Lund, unpublished.
11) S. Gupta and A. Irbäck, Phys. Lett. B286 (1992) 112.
12) M. Rao, H. R. Krishnamurthy and R. Pandit, Phys. Rev. B42 (1990) 856;
    W. S. Lo and R. A. Pelcovits, Phys. Rev. A42 (1990) 7471.