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# Droplet theory of low-dimensional Potts models

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**Abstract.** We formulate a generalisation of the droplet theory of Ising systems to droplet systems containing more than two phases, valid near one dimension and based on the configurational energy of surface tension. Thermal and magnetic exponents for these multi-phase systems are compared with the results for a  $q$ -state Potts model in an external field. The Potts exponents are obtained using a Migdal recursion formula and are shown to be of very similar structure.

## 1. Introduction

There has been considerable interest in droplet models in the area of critical phenomena. The ‘classical’ droplet picture was formulated by Becker and Döring (1935); a detailed description can be found in Frenkel (1955). Andreev (1963) and Fisher (1967) pointed out that the droplet model for condensation gives rise to an essential singularity of the free energy on the coexistence curve. Further studies and references are contained e.g. in the papers by Langer (1967), Domb (1976), Binder (1976) and Binder and Stauffer (1976).

We shall use a droplet model as a possible approach to investigate the behaviour of Ising-like systems, especially near the critical point. Bruce and Wallace (1981), hereafter referred to as BW, presented a droplet description of Ising systems with the Hamiltonian given in terms of surface area. This intuitively very straightforward model gives rise to considerable insight into how basic physical quantities, such as dimensionality and critical droplet concentration, govern exponent values.

In this paper, after reviewing the results for the two-phase model needed for the following, we generalise the description to multi-phase systems. In our framework this should provide an analogy to a Potts model (Potts 1952) with an appropriate number of spin states.

To check this conjecture we derive a Migdal–Kadanoff recursion formula (Migdal 1975/76, Kadanoff 1976) for the Potts model in an external field. As this renormalisation group scheme becomes exact in the limit  $d = 1$  we expect it to provide a good approximation in our case.

We find that the thermal and magnetic exponents obtained via these two approaches are very closely related to one another. In particular, they agree in those orders where the results of the Migdal scheme are independent of the scale transformation parameter  $p$ .

Furthermore, we analyse the diluteness approximation made by BW in neglecting partial droplet overlap. In the multi-phase system this approximation breaks down if the number of phases becomes very large for fixed dimension. Taking the same

limit in the Potts model changes its critical behaviour from a continuous to a discontinuous phase transition. With a view to the analogies between the Potts and the droplet models, we take the breakdown of the diluteness approximation as a sign for a similar change in the critical behaviour of the droplet model; i.e. we expect the droplet transition to turn first order for a sufficiently large number of phases.

## 2. The droplet model for multi-phase systems

Let us begin by reviewing the major results for the two-phase system as obtained by BW. The Ising-type model is set up by specifying the Hamiltonian governing the statistical mechanics of a single 'spin-up' droplet of a certain scale size  $R$  in homogeneous 'spin-down' phase. It is given in terms of surface area where the droplet is allowed to deviate from spherical by an amount  $f(\eta)$  in the direction  $\eta$  ( $L_{ij} = x_i \partial/\partial x_j - x_j \partial/\partial x_i$ ):

$$\mathcal{H} = \frac{1}{T_0} \int d\Omega (R+f)^{d-1} \left( 1 + \frac{1}{2}(R+f)^{-2} \sum_{i,j} (L_{ij}f)^2 \right)^{1/2}. \quad (2.1)$$

BW use this Hamiltonian to derive an expression for the mean fraction of available space occupied by all droplets of 'spin-up' phase with scale size between  $R$  and  $R+dR$  in  $d = 1 + \varepsilon$  dimensions:

$$\psi(R) dR = \frac{2}{\pi} (T(R))^{-(2+\varepsilon)/2} \frac{1}{R} \exp\left(-\left(\frac{S_d}{T(R)} - \frac{S_d^\nu}{T_c} + \frac{2}{\varepsilon\Gamma(d)}\right) dR [1 + O(\varepsilon, T(R))]\right). \quad (2.2)$$

Here  $\nu$  is the correlation length exponent obtained as

$$\nu^{-1} = \varepsilon + \frac{1}{2}\varepsilon^2 + O(\varepsilon^3) \quad (2.3)$$

and  $T_c$  denotes the critical temperature:

$$T_c = \varepsilon + O(\varepsilon^2). \quad (2.4)$$

$T(R)$  is an appropriate renormalised temperature which exhibits a crossover from large  $R$  behaviour:  $T(R) \sim (R/\xi)^{-\varepsilon}$ , to small  $R$  behaviour:  $T(R) \rightarrow T_c$ . The correlation length  $\xi$  provides the physical length scale of the theory which controls the crossover.

For  $R \gg \xi$ ,  $\psi(R)$  behaves as

$$\psi(R) \sim (R/\xi)^{\varepsilon(2+\varepsilon)/2} (1/R) \exp[-S_d(R/\xi)^\varepsilon] \quad (2.5)$$

where the exponential contains the surface area of a large droplet. In the following calculations,  $\psi(R)$  can therefore be neglected in this limit.

For  $R \ll \xi$ ,  $\psi(R)$  behaves as

$$\psi(R) = \psi_0 R^{-1} \quad (2.6)$$

the prefactor  $\psi_0$  being

$$\psi_0 = (2/\pi) \varepsilon^{-(2+\varepsilon)/2} \exp[-(1+2C+2/\varepsilon)][1+O(\varepsilon)] = A(e^{-2/\varepsilon}/\varepsilon)[1+O(\varepsilon)] \quad (2.7)$$

where  $C = 0.577 \dots$  is Euler's number and  $A$  summarises all the constants.

In order to construct multi-droplet configurations in a system allowing for more than two phases we start from a volume of scale size  $L$  occupied homogeneously by phase 1, say. It is decorated successively with droplets of all other phases and smaller

scale sizes down to a minimum scale size  $L_0$  which plays the role of the lattice spacing. For each phase the amount of volume used at every step of the procedure is given by the same function  $\psi(R)$ .

Thus each phase is assumed to have the same surface energy per unit surface area relative to any other phase. This leads us naturally to the Potts model as the appropriate spin model counterpart. In the  $q$ -state model the  $q$  spin vectors  $\sigma^\alpha$ ,  $\alpha = 1, \dots, q$ , point to the vertices of a hypertetrahedron in  $(q - 1)$ -dimensional space. Consequently, there are only two different values for the interaction energy possible which we normalise in the following way:

$$E(\sigma^\alpha, \sigma^\beta) = -K\delta(\sigma^\alpha, \sigma^\beta) = \begin{cases} -K, & \sigma^\alpha = \sigma^\beta \\ 0, & \sigma^\alpha \neq \sigma^\beta \end{cases} \quad \alpha, \beta = 1, \dots, q \quad (2.8)$$

with  $K > 0$  being the bond strength. Note that in this normalisation the standard Ising coupling  $K_I$  is given as  $K_I = K/2$ .

One can now use the decoration procedure sketched above to calculate the volume fraction  $\Psi_0(L, L_0)$  occupied by all outermost droplets of one phase  $k$ ,  $k = 2, \dots, q$  (outermost 1-droplets are of course nonsensical in this context). Let us assume that we have already decorated down to scale size  $R$ . In order to derive a differential equation for  $\Psi_0(L, R)$  we ask for the change  $d\Psi_0(L, R)$  which occurs if the decoration procedure is carried out one step further to include droplets of scale size  $R + dR$ , where  $dR < 0$ . We find

$$d\Psi_0(L, R) = -[1 - (q - 1)\Psi_0(L, R)]\psi(R) dR. \quad (2.9)$$

The term in square brackets contains the volume fraction which is available for the next step of the decoration procedure, i.e. which is not yet occupied by outermost droplets. The fraction of this volume which is actually used in the next step is given by  $\psi(R) dR$ . The minus sign has to appear because  $dR < 0$  but  $d\Psi_0(L, R) > 0$ .

Integrating from  $L_0$  up to  $L$  such that outermost droplets of all scale sizes between  $L_0$  and  $L$  are included yields

$$\Psi_0(L, L_0) = \frac{1}{q - 1} \left[ 1 - \exp\left(- (q - 1) \int_{L_0}^L \psi(R) dR\right) \right]. \quad (2.10)$$

The volume fraction occupied by all outermost droplets of all phases is

$$\Psi_0^T(L, L_0) = (q - 1)\Psi_0(L, L_0). \quad (2.11)$$

Similarly, to derive the total volume fraction  $\Psi(L, L_0)$  covered by  $k$ -phase ( $k = 2, \dots, q$ ), we ask again for an appropriate differential equation. We assume as before that the decoration procedure has already been carried out down to scale size  $R$ . Let us now decorate with droplets of all phases of scale size  $R + dR$ ,  $dR < 0$ . One finds two contributions to the change  $d\Psi(L, R)$  of the volume occupied by the single phase  $k$ :

$$d\Psi(L, R) = -[1 - \Psi(L, R)]\psi(R) dR + (q - 1)\Psi(L, R)\psi(R) dR. \quad (2.12)$$

With the same sign convention as before, the first term describes a gain in the volume occupied by  $k$ -phase. This is caused by decorating the volume occupied by all other phases with droplets of  $k$ -phase. The second term reflects a loss in  $k$ -volume, when it itself is decorated with droplets of the other  $(q - 1)$  phases.

Integrating from  $L_0$  to  $L$  yields

$$\Psi(L, L_0) = \frac{1}{q} \left[ 1 - \exp\left(-q \int_{L_0}^L \psi(R) dR\right) \right]. \quad (2.13)$$

The corresponding volume fraction for 1-phase is given by

$$\Psi^{(1)}(L, L_0) = 1 - (q-1)\Psi(L, L_0) = \frac{1}{q} \left[ 1 + (q-1) \exp\left(-q \int_{L_0}^L \psi(R) dR\right) \right]. \quad (2.14)$$

To calculate the mean number  $N(R)dR$  of  $k$ -phase droplets ( $k = 2, \dots, q$ ) with scale size between  $R$  and  $R + dR$  we first have to find the total volume occupied by these droplets and then divide it by the volume of a single droplet of scale size  $R$ . The total occupied volume is given by the product of the available volume and the function  $\psi(L, R)$  which tells us what fraction of it is in fact occupied. Obviously, the available volume is the volume which is not yet occupied by larger  $k$ -phase droplets, so that we find

$$N(R) = (L/R)^d [1 - \Psi(L, R)] \psi(R) \quad (2.15)$$

and by similar reasoning

$$N^{(1)}(R) = (L/R)^d (q-1) \Psi(L, R) \psi(R) = (L/R)^d [1 - \Psi^{(1)}(L, R)] \psi(R). \quad (2.16)$$

It is now possible to calculate the critical droplet density  $\rho_c$ . This quantity has to remain small in order to ensure the diluteness approximation contained in the derivation of (2.2). Using equations (2.15) and (2.16) we find

$$\rho_c = \left(\frac{L_0}{L}\right)^d \int_{L_0}^L [(q-1)N(R) + N^{(1)}(R)] dR = L_0^d (q-1) \int_{L_0}^L dR \frac{\psi(R)}{R^d}. \quad (2.17)$$

In the critical limit the correlation length  $\xi$  is very much larger than the lattice spacing  $L_0$  though still less than the system size  $L$ . We split the above integral into two parts ranging from  $L_0$  to  $\xi$  and from  $\xi$  to  $L$ . The second part is neglected because of the large  $R$  behaviour of  $\psi(R)$ ; in the first part  $\psi(R)$  is replaced by its small  $R$  limit. Neglecting the contribution from the upper end of this integral as well, one finally has

$$\rho_c = L_0^d (q-1) \psi_0 \int_{L_0}^{\xi} dR R^{-(d+1)} = \frac{(q-1)\psi_0}{d}. \quad (2.18)$$

It is clear from this expression and the preceding discussion that the number of phases must remain smaller than a certain maximum number  $q_{\max}$ . Choosing a suitably small value for  $\rho_c$  and inserting equation (2.7) for  $\psi_0$  yields for  $q_{\max}$

$$q_{\max} \sim (\rho_c/A) \varepsilon e^{2/\varepsilon}. \quad (2.19)$$

Hence the maximum allowed number of phases can only be increased if at the same time  $d$  approaches 1.

In order to find the net magnetisation of the system one has to specify the magnetisation contained in a droplet of phase  $k$  per unit volume. In straightforward generalisation of the Ising case we define the magnetisation as the sum over the  $q$  Potts spin vectors, each multiplied by the volume fraction occupied by the corresponding phase:

$$\mathbf{m}^{(q)} = \boldsymbol{\sigma}^1 \Psi^{(1)}(L, L_0) + \Psi(L, L_0) \sum_{k=2}^q \boldsymbol{\sigma}^k. \quad (2.20)$$

In performing the sum we use a recursion relation giving the spin vectors of a  $q$ -state Potts model in terms of those of a  $(q - 1)$ -state model (Zia and Wallace 1975). The result reads

$$m^{(q)} = [1 - q\Psi(L, L_0)]\sigma^1 \tag{2.21}$$

where  $\sigma^1$  is the spin vector chosen to represent the original homogeneous phase. In the critical limit which is calculated in the same way as for  $\rho_c$ ,  $m^{(q)}$  takes the form

$$m^{(q)} = \exp\left(-q \int_{L_0}^{\xi} \psi_0 R^{-1} dR\right) = (\xi/L_0)^{-q\psi_0}.$$

Thus the exponent  $\beta$  is identified as

$$\beta = \nu q \psi_0 = Aq(e^{-2/\epsilon}/\epsilon^2)[1 + O(\epsilon)]. \tag{2.22}$$

All the results obtained so far agree with the results for the Ising-like droplet system if  $q = 2$ . This is a first check on our generalisation. As a second check we shall derive a Migdal–Kadanoff recursion relation for the Potts model and use it to calculate critical exponents. These will then be compared with the droplet results. Note that so far, only the calculation of  $\beta$  made use of Potts model features. All other quantities were obtained completely independent of any spin picture.

### 3. Migdal recursion relations

We apply the Migdal–Kadanoff scheme to a  $d$ -dimensional hypercubic lattice of Potts spins. The procedure consists of two steps which are performed consecutively in each spatial direction. Firstly, all bonds and on-site potentials along a particular lattice direction are shifted to the edges of a lattice hypercube containing  $p^d$  spins. Secondly, those spins which are now no longer coupled to their neighbours are decimated. Thus an anisotropy in the coupling is generated but its effect vanishes in the limit  $d = 1$ . Therefore, although our recursion relation originally refers to the direction of the first shift, this will not affect our results.

Performing the linear chain decimation for Potts spins in an external field shows that the renormalisation group equations only close if we introduce a third coupling  $J$  in the Hamiltonian:

$$\begin{aligned} \mathcal{H} = -\sum_i \{ & K\delta(\sigma(i), \sigma(i+1)) + \frac{1}{2}h[\delta(\sigma(i), \sigma^1) + \delta(\sigma(i+1), \sigma^1)] \\ & + J\delta(\sigma(i), \sigma(i+1))[\delta(\sigma(i), \sigma^1) + \delta(\sigma(i+1), \sigma^1)] \}. \end{aligned} \tag{3.1}$$

The external field is applied parallel to the direction of the spin vector  $\sigma^1$ . With our energy normalisation the field term thus produces contributions to  $\mathcal{H}$  only for those spins which are in the state  $\sigma^1$ . The same Hamiltonian arises if the Hamiltonian of a  $(q - 1)$ -state lattice gas Potts model (Blume *et al* 1971, Berker *et al* 1978, Nienhuis *et al* 1979) is transformed into a  $q$ -state Potts Hamiltonian by introducing the vacancies as an extra spin state (Wu 1982). In our case this extra spin state corresponds to the state  $\sigma^1$ .

To perform the decimation a transfer matrix approach proves useful. Eliminating  $p$  spins amounts to taking the  $p$ th product of the transfer matrix ( $T_{ij}$ ) where

$$T_{11}^{(1)} = A^{(1)} = e^{K+h+2J}, \quad T_{1\alpha}^{(1)} = T_{\alpha 1}^{(1)} = B^{(1)} = e^{h/2},$$

$$T_{\alpha\alpha}^{(1)} = C^{(1)} = e^K, \quad T_{\alpha\beta}^{(1)} = D^{(1)} = 1, \quad \alpha, \beta = 2, \dots, q; \alpha \neq \beta. \tag{3.2}$$

The elements of  $T^{(p)}$  can be expressed in terms of the elements of  $T^{(p-1)}$ ; solving this recursion with (3.2) as initialising conditions yields

$$\begin{pmatrix} A^{(p)} \\ B^{(p)} \\ C^{(p)} \\ D^{(p)} \end{pmatrix} = \frac{1}{q-1} (e^K - 1)^p \begin{pmatrix} 0 \\ 0 \\ q-2 \\ -1 \end{pmatrix} - \frac{\alpha_+^p}{R} \begin{pmatrix} \frac{2(q-1)e^h}{W-R} \\ -e^{h/2} \\ \frac{W-R}{2(q-1)} \\ \frac{W-R}{2(q-1)} \end{pmatrix} + \frac{\alpha_-^p}{R} \begin{pmatrix} \frac{2(q-1)e^h}{W+R} \\ -e^{h/2} \\ \frac{W+R}{2(q-1)} \\ \frac{W+R}{2(q-1)} \end{pmatrix},$$

$$\alpha_{\pm} = \frac{1}{2}(e^{K+h+2J} + e^K + q - 2 \pm R),$$

$$R = [W^2 + 4(q-1)e^h]^{1/2}, \quad W = e^{K+h+2J} - e^K - (q-2). \tag{3.3}$$

Including the shift of the couplings as discussed above, the full Migdal-Kadanoff recursion relation is given as

$$\frac{K'}{p^{d-1}} = \ln \frac{C^{(p)}}{D^{(p)}}, \quad \frac{h'}{2p^{d-1}} = \ln \frac{B^{(p)}}{D^{(p)}},$$

$$\frac{2J'}{p^{d-1}} = \ln \left[ \frac{A^{(p)}}{C^{(p)}} \left( \frac{D^{(p)}}{B^{(p)}} \right)^2 \right]. \tag{3.4}$$

The fixed point of interest is the zero-field fixed point where  $h^* = J^* = 0$  holds exactly, and  $K^*$  obeys the equation

$$\exp(-K^*/p^{d-1}) = p \exp(-K^*) + (q-2) \binom{p}{2} \exp(-2K^*) + O[\exp(-3K^*)]. \tag{3.5}$$

Higher orders may be neglected because for  $d$  close to 1 we expect  $K^*$  to be very large, its inverse approaching the zero-temperature fixed point when  $d$  goes to 1.

Solving (3.5) to first order we have

$$K^* = 1/\varepsilon + O(1) \tag{3.6}$$

which confirms our expansion in  $\exp(-K^*)$ . Moreover, it is found to be in accordance to first order with expression (2.4) for the critical temperature in the droplet picture.

It is now straightforward to obtain critical exponents, e.g.

$$\nu^{-1} = \varepsilon + \frac{p-1}{\ln p} \left( \frac{q-2}{2} \exp(-K^*) + O[\exp(-2K^*)] \right). \tag{3.7}$$

Comparison with (2.3) again shows agreement in first order. In particular, neither  $K^*$  nor  $\nu$  show any  $q$ -dependence in first order. The magnetic exponent  $y_H$  reads

$$y_H^{-1} = d - \frac{p^2-1}{6 \ln p} q \exp(-2K^*) + O[\exp(-3K^*)]. \tag{3.8}$$

Using scaling laws we obtain

$$\begin{aligned}\beta &= \nu(d - y_H^{-1}) = \frac{p^2 - 1}{6 \ln p} \frac{q}{\varepsilon} \exp\left[-2\left(\frac{1}{\varepsilon} + O(1)\right)\right] [1 + O(e^{-1/\varepsilon})] \\ &= C \frac{p^2 - 1}{6 \ln p} \frac{q}{\varepsilon} e^{-2/\varepsilon} [1 + O(e^{-1/\varepsilon})],\end{aligned}\quad (3.9)$$

where the  $O(1)$  terms are contained in the constant  $C$ .

The comparison with our previous result equation (2.22) for  $\beta$  shows that in both cases the first non-vanishing term in an  $e^{-1/\varepsilon}$  expansion of  $\beta$  appears in order  $e^{-2/\varepsilon}$ .

Note that we recover the same  $q$ -dependence as before. We cannot, of course, expect exactly the same prefactor structure. Firstly, this would require an explicit expression of the  $O(1)$  terms in equation (3.6) for  $K^*$ ; and secondly, even then the prefactor has to be treated with some care as it depends on the scale parameter  $p$ . However, as usual in the Migdal scheme, the singularities which occur in the equations if we take  $p = 1$  cancel.

A very significant feature of the Potts model is the change of its critical behaviour from a continuous to a discontinuous phase transition. Mean-field theory predicts that the transition is first order for all  $q > 2$  independent of the dimensionality (Kihara *et al* 1954, Wu 1982 and references therein). This does not agree with the exact result for  $d = 2$  where the transition is first order only for  $q > 4$  (Baxter 1973). Consequently, a considerable amount of research has been carried out to determine the number of spin states  $q_c(d)$  above which, in  $d$  dimensions, the transition behaviour predicted by mean-field theory is found. For  $d \rightarrow 1$ ,  $q_c(d)$  approaches infinity as  $q_c(d) \sim e^{2/d-1}$  (Berker *et al* 1980, Nienhuis *et al* 1981). Recall that in the droplet discussion the maximum allowed number of phases behaves as  $q_{\max} \sim \psi_0^{-1} \sim \varepsilon e^{2/\varepsilon}$  for small  $\varepsilon = d - 1$ . Because of the similarity of these two quantities and the analogies between the droplet and the Potts model obtained so far, one is tempted to extend the analogies further and conjecture a change from a continuous to a discontinuous phase transition in the droplet system if  $q > q_{\max}$ .

Let us conclude with a remark on the  $q = 1$  case. It has been shown (Kasteleyn and Fortuin 1969) that the problem of bond percolation on a lattice can be formulated in terms of the  $q = 1$  limit of the Potts model. A similar equivalence exists for site percolation (Giri *et al* 1977, Kunz and Wu 1978). Starting from the standard field theoretic description of the Potts model and taking the limit  $q = 1$ , Lubensky and McKane (1981) find a singularity in the free energy which has the same structure as the one found by Langer (1967) in his studies of metastability in the Ising model. In the same spirit, we can easily extend our results to account for the case  $q = 1$ . A physical interpretation of this formal limit, however, presents some difficulties. This is obvious from the decoration procedure used to construct multi-droplet (i.e. close to criticality) configurations. It starts with the system being in the fully ordered state which is well defined for the droplet model. For the percolation problem, however, a precise description of the ground state is still missing. Furthermore, the decoration procedure requires at least two phases: one which is originally homogeneously distributed in the system and another different phase which is used to start the decoration. With a view to these features, the relations between the configurational physics governing the percolation problem and the droplet framework certainly need further clarification.



#### 4. Concluding remarks

In order to describe Potts-like systems, we have presented two models: firstly, the problem was formulated in terms of droplets and their surface tension, and secondly, it was cast in a spin Hamiltonian form based on the interaction energy of neighbouring spin states. Although these two approaches originate from very different ideas, the respective results show apparent analogies. This provides a strong argument for the usefulness of surface tension droplet models in the area of critical phenomena.

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