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Wetting in Potts and Blume–Capel Models

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We discuss the wetting of the interface between two ordered phases by the disordered one in the Potts model with q large. We argue that a "low-temperature" expansion can be used in this situation, with $\log q$ replacing β. This model is analogous to the Blume–Capel model at low temperatures, which we use as an example to review the low-temperature expansions.

KEY WORDS: Wetting; surface tension; low-temperature expansion; large-q expansion.

1. INTRODUCTION

Wetting may occur when three or more phases (A, B, C,...) coexist. It consists of the appearance of a thick (macroscopic) layer of the C phase at an interface between the A and the B phases. This phenomenon has been observed experimentally and in computer simulation (for a review, see Ref. 1). It has also been investigated by mean field theory$^{(2-4)}$ and by low-temperature expansions.$^{(5,6)}$ In this note we use the method of low-temperature expansions$^{(7,8)}$ to analyze the wetting of two ordered phases by the disordered one in the q-state Potts model, for q large. We first review low-temperature expansions in a simple example: the (generalized) Blume–Capel model. There we make explicit the connection between these expansions and the rigorous Pirogov–Sinai theory of first-order phase transition.$^{(7,9)}$ We argue that the Potts model, at the transition temperature where ordered and disordered states coexist, is very similar, for large q, to the Blume–Capel model at low temperatures. Then we carry out for the

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Potts model a $q^{-1/d}$ expansion similar to the one done in $e^{-\beta}$ for the Blume–Capel model.

The criterion for deciding whether phase C wets an A–B interface is obtained by first computing the surface tensions between all possible interfaces, A–B, A–C, B–C. Then, if

$$\tau_{AB} > \tau_{AC} + \tau_{BC} \tag{1.1}$$

one expects a thick layer of the C phase to form itself at the A–B interface, while, if the reverse inequality holds, then the A–B interface should be thin. However, it is not immediately obvious how to define these surface tensions. Usually, e.g., in the Ising model, they are defined by imposing different boundary conditions (b.c.), say A on the top and B on the bottom of a large box, and then taking the difference between the free energy of that system and the average of the free energies with homogeneous b.c. (all A or all B). But, if wetting by the C phase does occur, then this A–B surface tension will actually equal $\tau_{AC} + \tau_{BC}$, so that the strict inequality in (1.1) never occurs for these "usual" tensions.

A similar problem occurs when one wants to compute a bulk phase diagram at low temperatures. Suppose that we have two possible phases, A and B; then one is supposed to compute the free energy of each phase and see which is the lowest. This gives the true thermodynamic phase; equality of these free energies yields the coexistence line. However, again, if one carries out an honest computation, one always obtains, independent of the b.c., the same (true) free energy in the thermodynamic limit.

Nevertheless, for the bulk phase diagram, the comparison between free energies has a well-defined meaning in (low-temperature) perturbation theory. One computes the free energy of a "gas" of low-energy excitations of each of the ground states up to certain order in a perturbation series. These free energies will depend, in general, on which ground state is considered. The scheme described above to find the true thermodynamic phase becomes meaningful when applied to these "restricted" free energies. This is reviewed in Section 2, in the special, but typical, case of the Blume–Capel model. We emphasize that, for the bulk phase diagram, this perturbative scheme can be entirely justified using the Pirogov–Sinai theory.(7,9)

In order to decide whether a given inteface is wetted or not by a third phase, we apply the same method as in the bulk, i.e., we associate to each interface a restricted surface tension that takes into account only the lowest energy excitations of the interface. This method has not been shown to be rigorous in this context (for some steps in this direction, see Ref. 10), but we feel quite confident that it gives the correct answers. We apply it first to the generalized Blume–Capel model (Section 2), and then to the Potts model for large q. There, we start by explaining why in the Potts model, the large-q limit can be regarded as a low-temperature limit, while β plays the role of an external field. Then the application of our method is straightforward. It yields results in accordance with those of other methods, i.e., at the transition point the interface between two ordered phases is wetted by the disordered, high-temperature phase. While previous results were obtained for q near 2,(2) or in two dimensions,(1,11) ours are relevant for q large and for three or more dimensions. In two dimensions, the interface is one-dimensional, and low-temperature expansions in one dimension are somewhat ill-defined (see remarks at the end of Section 2).

2. GENERALIZED BLUME–CAPEL MODEL

2.1. Low-Temperature Phase Diagram: Pirogov–Sinai Theory

At each site $x \in \mathbb{Z}^d$ $(d \geqslant 2)$, we have a "spin" variable S_x taking three values, -1, 0, and $+1$. The energy in a finite box Λ of a configuration S_Λ, given a b.c. S_{Λ^c} (i.e., a configuration outside Λ) is

$$H_\mu(S_\Lambda \mid S_{\Lambda^c}) = \sum_{\langle xy \rangle \cap \Lambda \neq \varnothing} |S_x - S_y|^\gamma - \mu \sum_{x \in \Lambda} S_x^2 \tag{2.1}$$

where $\gamma > 0$ ($\gamma = 2$ and $\gamma = 1$ being the cases most frequently considered).

The equilibrium state in Λ is given by the probability distribution

$$P(S_\Lambda \mid S_{\Lambda^c}) = Z^{-1}(\Lambda \mid S_{\Lambda^c}) \exp[-\beta H_\mu(S_\Lambda \mid S_{\Lambda^c})] \tag{2.2}$$

where β^{-1} is the temperature T and the partition function is

$$Z(\Lambda \mid S_{\Lambda^c}) = \sum_{S_\Lambda} \exp[-\beta H_\mu(S_\Lambda \mid S_{\Lambda^c})] \tag{2.3}$$

The free energy per spin

$$\psi(\beta, \mu) = \lim_{\Lambda \to \infty} -(\beta\, |\Lambda|)^{-1} \log Z(\Lambda \mid S_{\Lambda^c}) \tag{2.4}$$

is independent of S_{Λ^c}.

For μ equal zero in (2.1), the Hamiltonian H_0 has three ground states: $S_x = \alpha$, $\forall x \in \mathbb{Z}^d$, with $\alpha = -1, 0, +1$, while there are only two ground states ($+1$ and -1) for $\mu > 0$ and only one ($S_x = 0$) for $\mu < 0$.

It can be rigorously shown(7) (using the Pirogov–Sinai theory) that, at low temperatures, there exists a line $\mu_t(\beta)$, approaching zero as β goes to infinity, on which three pure phases coexist. (By pure phase we mean here a Gibbs state(12) that is translation-invariant and extremal, i.e., is not a combination of other Gibbs states). These phases are the limiting probability distributions obtained by letting $\Lambda \uparrow \mathbb{Z}^d$ in (2.2) with the b.c.

$S_x = +1$, $\forall x \in \Lambda^c$ (or $= -1$ or $=0$). Each of these states can be described as a small perturbation of the corresponding ground state. For example, for the state corresponding to $+1$, typical configurations will consist of a sea of $+1$ spins with small islands of the other phases (0 or -1).

For $\mu > \mu_t(\beta)$, there are two pure phases corresponding to the $+1$ and -1 ground states, while for $\mu < \mu_t(\beta)$, we have only one pure phase, corresponding to the 0 ground state. The magnetization of the $+1$ or -1 phases jumps discontinuously across $\mu_t(\beta)$ and the transition there is of first order. This is the rigorous picture at low temperatures. For higher temperatures the transition is expected to become of second order (see Fig. 1). Here, we shall restrict our attention to small μ and small temperatures, i.e., to the first-order transition.

Let us now review how one computes in perturbation theory the equation of the line $\mu_t(\beta)$. Before doing this, we emphasize that the Pirogov–Sinai theory is much deeper than the perturbative argument given below (which is a somewhat streamlined version of standard methods[7,8]). It actually gives a completely rigorous description of the phase diagram for β large. Using this theory, one shows that the perturbation theory gives indeed the correct asymptotic expansion of $\mu_t(\beta)$ as $\beta \to \infty$.[7]

We define an *excitation* of a ground state as a configuration that coincides with this ground state outside a finite region. The support of an excitation (i.e., the complement of the infinite connected set where the configuration coincides with the ground state) can be decomposed into con-

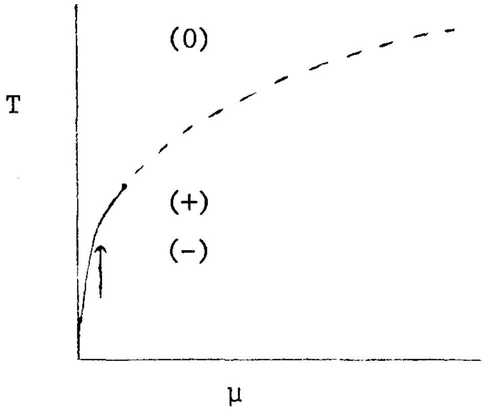


Fig. 1. Phase diagram of the Blume–Capel model, $d=2$, $\gamma=2$ (adapted from Ref. 1, Fig. 3). The line is $T_t(\mu)$ [equivalently, $\mu_t(\beta)$], on which three phases coexist. For $T < T_t(\mu)$, there are two phases ($+$ and $-$), while there is only one phase (0) above $T_t(\mu)$. The solid part of the line corresponds to a first-order transition, while the dotted part is a second-order transition. The arrow is the line $T \uparrow T_t(\mu)$ considered in Section 2.2.

nected components. The restriction of an excitation to such a component is called an *elementary excitation.* Let us consider the set of excitations $\Omega(E)$ for which each elementary component has an energy, computed with the Hamiltonian H_0, (2.1), less than or equal to E. Observe that, for any fixed E, the support of an elementary excitation is bounded. This property, which is shared by many systems but not, e.g., by the one-dimensional Ising model, is called *regularity* of the Hamiltonian and is essential for this perturbative analysis to work. $\Omega(E)$ is the configuration space of a "gas" of elementary excitations that feel a hard-core exclusion, since the supports of different excitations have to be disjoint from each other. If we take, for example, $E=2d$, then the elementary excitations of the 0 ground state correspond to isolated $+1$ spins or -1 spins surrounded by 0 spins, and the excitations of the $+1$ ground state correspond to 0 spins surrounded by $+1$ spins (-1 spins are not permitted at this order because their energy is $2^\gamma 2d > 2d$). Let

$$Z_\alpha^E(\Lambda, \beta, \mu) = \sum_{S_\Lambda}{}^E \exp[-\beta H_\mu(S_\Lambda \mid \alpha)] \tag{2.5}$$

where the sum is restricted to the gas of elementary excitations of the ground state α and we have b.c. $S_x = \alpha$, $x \in \Lambda^c$. For example,

$$Z_0^{2d}(\Lambda, \beta, \mu) = \sum_{S_\Lambda}{}^{2d} \exp[-\beta(N_+ + N_-)(2d-\mu)]$$

where $N_+ = N_+(S_\Lambda)$ (resp. N_-) is the number of elementary excitations consisting of isolated $+1$ spins (resp. -1 spins). On the other hand,

$$Z_+^{2d}(\Lambda, \beta, \mu) = [\exp(\beta\mu \mid \Lambda \mid)] \sum_{S_\Lambda}{}^{2d} \exp[-\beta N_0(2d+\mu)]$$

where N_0 is the number of isolated 0 spins, and $Z_-^{2d} = Z_+^{2d}$, by symmetry.

The thermodynamic limit of the free energy of the gas of elementary excitations

$$\psi_\alpha^E(\beta, \mu) = \lim_{\Lambda \to \infty} -(\beta \mid \Lambda \mid)^{-1} \log Z_\alpha^E(\Lambda, \beta, \mu) \tag{2.6}$$

exists, by the usual subadditivity arguments, for any β and μ.

In the above examples, we obtain for β large and $|\mu| < 2d$

$$\psi_0^{2d}(\beta, \mu) \approx -\frac{2}{\beta} \exp[-\beta(2d-\mu)] \tag{2.7}$$

$$\psi_+^{2d}(\beta, \mu) = \psi_-^{2d}(\beta, \mu) \approx -\mu - \frac{1}{\beta} \exp[-\beta(2d+\mu)] \tag{2.8}$$

In general, there exists, for any fixed E, constants $\mu(E)$ and $\beta(E)$ such that, for $|\mu| < \mu(E)$ and $\beta > \beta(E)$, $\psi_\alpha^E(\beta, \mu)$ is equal to the energy of the ground state α, plus a convergent series in a finite number of variables $(1/\beta) \exp[-\beta E_i(\mu)]$, where $E_i(\mu)$ denotes the energy of the ith excitation as a function of μ. [We emphasize that the excitations are ordered so that $E_1(0) < E_2(0) < \cdots$.] For a proof of convergence, see Ref. 7. In general, one expects the convergence to be nonuniform in E.

The transition line $\mu_t(\beta)$ is obtained by solving the equation

$$\psi_+^E(\beta, \mu) = \psi_-^E(\beta, \mu) = \psi_0^E(\beta, \mu) \tag{2.9}$$

where the first equality holds by symmetry. This yields $\mu_t(\beta)$ up to an error of order $o(e^{-\beta E})$. From (2.7)–(2.9) we find that, to first order, $\mu_t(\beta) \approx (1/\beta) \exp(-2d\beta)$, independent of γ.

Remark. For fixed E, ψ_α^E is well-defined for all μ and β. In particular, ψ_+^E is defined for values of μ where the only pure phase corresponds to the 0 ground state, i.e., $\mu < \mu_t(\beta)$, and vice versa. It is natural to ask: What is the exact meaning of ψ_+^E for those values of μ? It cannot be equal or close to the thermodynamic limit of the free energy defined with $+1$ b.c., since this limit is independent of the b.c. In fact, ψ_0^E would be equal, up to terms of order $e^{-\beta E}$, to the true free energy. It cannot be said either that $\psi^E(+1)$ is the analytic continuation of the true free energy, starting from the region $\mu > \mu_t(\beta)$, because such an analytic continuation is, in general, impossible (see Ref. 13 for rigorous results). We do not in fact have any precise answer to the above question; it is presumably related to the "metastable free energy" of the $+$ phase. All we can say at present is that ψ_α^E for $\mu \neq \mu_t(\beta)$ is a convenient tool to compute the transition line.

2.2. Interfaces and Wetting

Let us fix $\mu > 0$ small and let the temperature be raised, starting from zero. Then we have two pure phases, $+1$ and -1, and we reach a first-order transition at a temperature T_t [such that $\mu = \mu_t(\beta_t)$] where the three phases coexist and above which only the 0 phase is present (see Fig. 1).

In order to study interfaces, one introduces the $+/-$ b.c.: Put $s_x = +1$ on the upper half of the boundary of a rectangular box Λ and $s_x = -1$ on the lower half. Then we ask: what state is obtained in the thermodynamic limit with these b.c.? For T small, the answer is known and depends on the dimension. For $d \geqslant 3$, a "rigid" interface will separate the space into a $+1$ phase and a -1 phase.(14,15) For $d = 2$, however, the interface, being a line, will fluctuate "out of sight," and the resulting state will be a convex combination of the $+1$ and -1 phases.(16–18) It is important to realize that, despite these fluctuations, the interface is locally very sharp at low temperatures and separates the $+1$ spins from the -1 spins; in particular, there are very few 0 spins (this can be proven using the method of Ref. 19).

The question that we try to answer now is: what happens when $T \uparrow T_t$? Two scenarios are possible: (a) the interface between the $+$ and the $-$ phases remains sharp us to T_t (locally sharp if $d = 2$) or, (b) the interface is "wetted" by the 0 phase, i.e., a thick layer of the 0 phase, whose thickness diverges as $T \uparrow T_t$, separates the $+$ and the $-$ phases. At T_t itself, one would then obtain the pure 0 phase in the thermodynamic limit with these $+/-$ b.c. In case (b) a next question is: how does the thickness of the 0 layer diverge? In particular, does this happen continuously, or through a sequence of layering transitions?(20,3,5,6)

We have no rigorous answer to these questions at the present time. However, as we have just seen, the bulk properties can be rigorously decided on the basis of a perturbative calculation, using restricted free energies. We propose to do a similar calculation with free energies associated to the different interfaces, i.e., with surface tensions.

To carry out this program, we must find out which interfaces will be the ground states, in the thermodynamic limit, when we impose $+/-$ b.c. The answer depends on γ: For $\gamma < 1$, there is just one ground state, given by a flat $+/-$ interface, while for $\gamma > 1$ the ground state is infinitely degenerate, with $n \geqslant 1$ number of layers of 0 spins. For $\gamma = 1$, we can have both situations: a sharp $+/-$ interface or several layers of 0 spins. Let us see what happens to these ground-state interfaces along the transition line, $\mu_t(\beta)$. For $\gamma < 1$, one expects the $+/-$ interface to remain sharp at low temperatures (this can probably be proven using the methods of Ref. 15). For $\gamma > 1$, the thickness of the layer of 0 spins would tend to infinity in the thermodynamic limit, because of the entropic repulsion between the interface separating the $+$ and the 0 spins, and the one separating the 0 and the $-$ spins. This entropic repulsion can be analyzed in terms of a gas of low-energy excitations of these interfaces, in a way similar to the one followed here.(10) Thus, the delicate point is $\gamma = 1$. In order to do as in the bulk, we introduce a surface tension of low-energy excitations of the interfaces.

Let us first define the "true" thermodynamic surface tensions between the different phases:

$$\tau_{\alpha,\delta}(\beta, \mu) = \lim_{L \to \infty} -(\beta L^{d-1})^{-1} \log \frac{Z(\Lambda \mid \alpha, \delta)}{[Z(\Lambda \mid \alpha)\, Z(\Lambda \mid \delta)]^{1/2}} \tag{2.10}$$

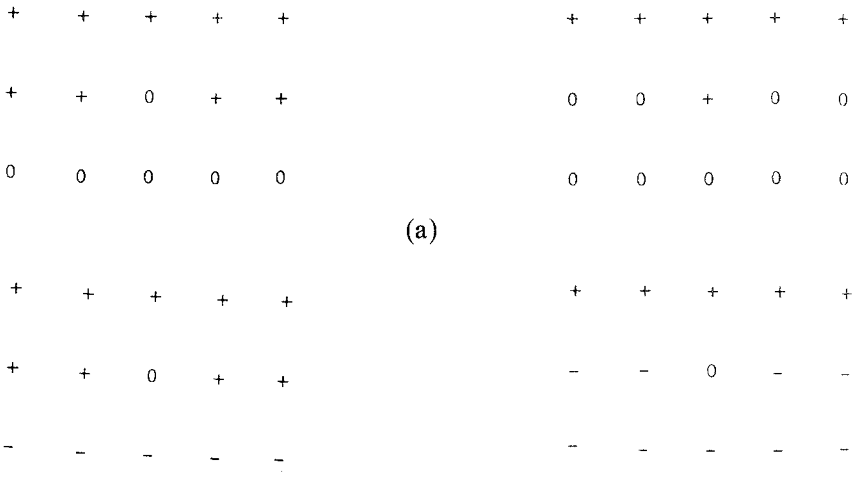
where $|\Lambda| = L^d$ and where $Z(\Lambda \mid \alpha, \delta)$ is the partition function in Λ with α b.c. on top and δ b.c. on the bottom of Λ. The two other partition functions have homogeneous b.c., all α, or all δ; $\alpha, \delta = +1, 0, -1$; $\alpha \neq \delta$. Now we define the corresponding restricted partition function $Z^E_{\alpha,\delta}(\Lambda)$ by summing only over configurations that coincide with a sharp α/δ interface outside Λ and differ from the α/δ ground state only on connected sets where the energy of an elementary excitation does not exceed E. The restricted surface tension $\tau^E_{\alpha,\delta}(\beta, \mu)$ is defined with this partition function, and with $Z^E_\alpha(\Lambda)$ and $Z^E_\delta(\Lambda)$, defined in (2.5), inserted in (2.10). We now compute these restricted surface tensions, and if we find, as the computation below does, that

$$\tau^E_{+,-}(\beta, \mu_t) > \tau^E_{+,0}(\beta, \mu_t) + \tau^E_{0,-}(\beta, \mu_t) = 2\tau^E_{+,0}(\beta, \mu_t)$$

for some E and large β, then we expect that the $+/-$ interface will be wetted by an infinite layer of the 0 phase at low temperatures. If the reverse inequality was to hold, then one would expect the $+/-$ interface to remain sharp even when all three phases coexist. Observe that, if the inequality holds in some direction for some E as $\beta \to \infty$, then it also holds for $E' > E$ in the same limit, since the inclusion of excitations of energy larger than E only modifies the free energies by terms $o(e^{-\beta E})$.

For $\tau^E_{+,0}$, in $d \geqslant 3$, one sees that the lowest energy excitations $[E = 2(d-1)]$ correspond to the insertion of either a 0 spin in the + half-space, or a + spin in the 0 half-space (see Fig. 2a). Thus,

$$\beta\tau^E_{+,0} \approx \beta - 2\exp[-2(d-1)\beta]$$


(a)

(b)

Fig. 2. Lowest energy excitations of the interfaces in the Blume–Capel model ($\gamma = 1$): (a) $+/0$ interface; (b) $+/-$ interface.

[since $\mu_t(\beta) \approx \exp(-2d\beta)$, it can be neglected at this order, and so can the excitations of Z_γ^E, Z_δ^E, which are of order $\exp(-2d\beta)$]. For $\tau_{+,-}^E$, one may insert a 0 spin either in the + or in the − half-space (see Fig. 2b). The insertion of a + spin in − spins or vice versa costs a higher energy. Thus,

$$\beta\tau_{+,-}^E \approx \beta - 2\exp[-2(d-1)\beta]$$

and

$$\beta(2\tau_{+,-}^E - \tau_{+-}^E) \approx -2\exp[-2(d-1)\beta] < 0$$

We expect, therefore, that at least for small μ and T, an infinite layer of the 0 phase will wet the +/− interface at T_t.

Remark 1. What happens in two dimensions? There the interface is really a one-dimensional system; it is (therefore) not a regular system, i.e., there are too many excitations with a given energy corresponding to steps in the interface and there is no convergent expansion for the gas of low-energy excitations, at least not any obvious one. So, strictly speaking, the method outlined above does not work for $d = 2$. However, our calculation still suggests that one gains entropy by inserting layers of 0 spins, so we expect a similar result. This is certainly true for $\gamma > 1$, where one gains energy. This model provides a nice illustration of the difference between wetting and roughening: For $T < T_t$, the +/− interface will be sharp, but, since it is a line, it will fluctuate widely, so that in the thermodynamic limit one obtains a Gibbs state that is a convex combination of the + and the − phases. On the other hand, at $T = T_t$, the same b.c. will lead to the pure 0 state.

Remark 2. Let us emphasize some differences between the cases $\gamma > 1$ and $\gamma = 1$. In both situations wetting is expected to occur because the (restricted) free energy of a +/− interface is higher than the combined free energies of +/0 and a 0/− interface. However, for $\gamma > 1$, say $\gamma = 2$, the difference between these free energies is due to the ground state and is of order one (per unit surface area), while for $\gamma = 1$ it is due to low-energy excitations and is of order $(1/\beta)\, e^{-c\beta}$ for some $c > 0$, as we have just seen.

This has two consequences: First, for $\gamma > 1$, there will be, even for T much below T_t, one (or several) layers of zeros, while for $\gamma = 1$ this is much less likely. Thus, the divergence of the width W_0 of the layer of zeros should occur only for T very close to T_t when $\gamma = 1$. Second, since the free energy difference that is responsible for this divergence is small, we expect it to be difficult to observe in numerical simulations because of boundary effects. This is especially true at low temperatures, even though the correlation length is small there, and one might think that finite-size effects are small, too.

So we expect that a numerical simulation for $\gamma = 1$ would give different results than the one done for $\gamma = 2$.[11] However, we see no theoretical reason why the true asymptotic divergence (in infinite volume, when $T \uparrow T_t$) of $W_0(T)$ should be different for $\gamma = 1$ or $\gamma = 2$. Rather, we conjecture that the scaling theory[25] relating W_0 to the ground state of a Schrödinger operator via a Feynman–Kac formula also applies to $\gamma = 1$; this implies that we expect a divergence of the form $W_0(T) \approx |T - T_c|^{-1/3}$. This remark may be relevant to understanding the numerical data obtained for the Potts model,[1] as we shall discuss in the next section.

3. THE POTTS MODEL

3.1. Phase Diagram

At each site $x \in \mathbb{Z}^d$ we have a variable $S_x = 1,\ldots, q$ and the Hamiltonian is given by

$$H(S_A) = -\sum_{\langle xy \rangle} \delta(S_x - S_y) \tag{3.1}$$

where $\delta(\cdot) = 0$ or 1 is the Kronecker delta. (Boundary conditions, equilibrium states, etc., can be introduced as in Section 2.)

It is known[21,22] that, for q large enough, the phase diagram is as follows: For β large, there are q pure phases, with most spins in each phase equal to one of the q possible values. At high temperatures, there is only one phase, the disordered one. The transition between the two regimes is of first order: At β_t ($\sim d^{-1} \log q$) the energy $[= \langle \delta(S_x - S_y) \rangle]$ and the "magnetization" $[= \langle \delta(S_x - m) \rangle$ in the mth phase$]$ are discontinuous.

For q large and $\beta > \beta_t$, mixed b.c. ($S_x = r$ on the top, $S_x = m \neq r$ on the bottom) produce a non-translation-invariant state if $d \geqslant 3$ or a fluctuating, but (locally) sharp, interface if $d = 2$. The question is whether this interface is wetted by the disordered phase at β_t. While discussing this, we shall not consider the way in which this layer of disordered phase increases in thickness as T approaches T_t.

Before carrying out the analysis, we shall argue that this model is, for q large, very similar to the Blume–Capel model for β large. Then we shall perform a perturbative calculation in $q^{-1/d}$ for the wetting problem, which will be the analogue of the low-temperature expansion of the preceding section.

To do this, we rewrite the model in a form that makes the analogy with the Blume–Capel model more transparent. For each bond $\langle xy \rangle$, we introduce a variable $t_{xy}=\delta(S_x-S_y)=0$ or 1. The partition function can be rewritten as

$$Z(\Lambda)=\sum_{S_\Lambda}\exp\left[\beta\sum_{\langle xy\rangle}\delta(S_x-S_y)\right]=\sum_{t_{xy}=0,1}\exp\left[\sum_{\langle xy\rangle}\beta t_{xy}+S(t_\Lambda)\right] \tag{3.2}$$

where $S(t_\Lambda)=\log$(number of configurations consistent with a given assignment of $\{t_{xy}\}$). Of course, this number may be zero, in which case we say that the configuration of the t variables is not admissible, and we restrict the sum in (3.2) to admissible configuration. $S(t_\Lambda)$ may be considered as an entropy term, but we shall consider it below as an energy term. Let $\beta=\tilde{\beta}\log q$ and define

$$-\tilde{H}(t_\Lambda)=\tilde{\beta}\sum_{\langle xy\rangle}t_{xy}+S(t_\Lambda)/\log q \tag{3.3}$$

Then

$$Z(\Lambda)=\sum_{t_{xy}=0,1}^{*}\exp[-(\log q)\,\tilde{H}(t_\Lambda)] \tag{3.4}$$

the sum $\sum^*$ being over admissible configurations.

This representation calls for the following observations:

1. The number of values taken by the variables t_{xy} is reduced to two, uniformly in q. Moreover, the energy per bond is bounded uniformly in q, since it is easy to see that $0\leqslant S(t_\Lambda)\leqslant|\Lambda|\log q$ if t_Λ is admissible.

2. In (3.4), $\log q$ plays the role of β in the Blume–Capel model, while $\tilde{\beta}$ will play the role of μ. More precisely, one observes that, for $\tilde{\beta}=d^{-1}$, there are two "ground states" when $\log q\to\infty$, the configuration $t_{xy}=0$, $\forall xy$, and the one with $t_{xy}=1$, $\forall xy$. Indeed, when all the t variables are 0,

$$S(t_\Lambda)=[\log q+O(q^{-1})]\,|\Lambda|$$

while if all t's are $+1$, $S(t_\Lambda)=\log q$, but $\sum_{\langle xy\rangle}t_{xy}\approx d\,|\Lambda|$, as $\Lambda\to\infty$. So μ in the Blume–Capel model is replaced here by $\tilde{\beta}-d^{-1}$. There is a line $\tilde{\beta}_t(q)$, similar to $\mu_t(\beta)$, of first-order transitions on which two phases coexist, one with most t_{xy} variables equal to 1 and one with most equal to 0. From this point of view the degeneracy between the q phases is ignored. For $\beta\neq\beta_t$, there is only one phase. Of course, in the present interpretation, the model is somewhat peculiar, since the Hamiltonian contains a "temperature-dependent" term, i.e., $S(t_\Lambda)/\log q$ [it does depend on q and $(\log q)^{-1}$ is now playing the role of the temperature]. However, this dependence is weak for q large (of order $1/q$), and provided we take it into account in our calculations, it does not invalidate our method.

To illustrate what the low-energy excitations are in this model for the disordered phase, let us compute the first one: It is given by one $t_{xy}=1$, all other t's being 0. To leading order, one loses a factor of q in the "entropy" term, $\exp S(t_\Lambda)$, and one gains a factor $\exp \beta$ from the energy, so that this excitation has a weight $e^\beta/q \approx q^{(1-d)/d}$ for $\beta = d^{-1} \log q$. Just as in the Blume–Capel model, one may compute perturbatively $\tilde{\beta}_t(q)$ (see Ref. 23 or Ref. 24, where a more systematic but conceptually equivalent approach is used). One obtains to leading order

$$\beta_t = \tilde{\beta}_t \log q \approx d^{-1} \log q + q^{(1-d)/d}$$

3.2. Interfaces and Wetting

As in the Blume–Capel model, we introduce surface tensions and restricted surface tensions between any two phases of the model. By symmetry, we need only to consider them for two ordered phases, say 1 and 2, and for an ordered and the disordered phase, say 1–D. First of all, it should be clear that the "ground-state energy" of a 1–2 interface is twice that of a 1–D interface, so that we have essentially the same degeneracy here as in the Blume–Capel model for $\mu = 0$ and $\gamma = 1$ (an arbitrary number of layers of disordered bonds may be inserted between the 1 and the 2 phases). Indeed, for the 1–2 interface, the ground-state energy is just 1 (per unit of surface), since one bond in the interface is broken and no entropy is gained. In order to compute the "ground-state energy" of the 1–D interface, we consider a rectangle Λ, with Λ^0 being the top half, Λ^1 the bottom half. We denote by $|\Lambda|$ the number of sites in Λ, $|\Lambda| = 2\,|\Lambda^0| = 2\,|\Lambda^1|$, $\partial\Lambda = \{\langle xy\rangle \mid x \in \Lambda, y \in \Lambda^c\}$, $b(\Lambda)$ the number of bonds in Λ, $b(\partial\Lambda)$ the number of bonds in $\partial\Lambda$, and similarly for Λ^0, Λ^1. The common boundary $P = \partial\Lambda^0 \cap \partial\Lambda^1$ between the two subsets of Λ is called the interface and $b(P)$ is the number of bonds in P. In Λ^1 we have only the (ordered) ground state 1, and in Λ^0 we have only the disordered "ground state" (all $t_{xy} = 0$). The t_{xy}'s are also 0 across the interface. Let $Z^0_{1,D}(\Lambda)$ be the corresponding partition function, where the subscript 0 refers to the fact that we do not allow any "excitations" of the "ground states." $Z^0_1(\Lambda)$ [resp. $Z^0_D(\Lambda)$] is the corresponding partition function with the ground state 1 (resp. D) everywhere in Λ. Then we have

$$\begin{aligned}
\log Z^0_1(\Lambda) &= \beta[b(\Lambda) + b(\partial\Lambda)] \\
\log Z^0_D(\Lambda) &= \log S(t_{xy} = 0, \forall xy) \\
&= \left[\log q + O\left(\frac{1}{q}\right)\right] |\Lambda| + O\left(\frac{1}{q}\right) b(\partial\Lambda)
\end{aligned}$$

$$\log Z^0_{1,D}(\Lambda) = \beta[b(\Lambda^1) + b(\partial\Lambda^1) - b(P)] + \left[\log q + O\left(\frac{1}{q}\right)\right] |\Lambda^0| + O\left(\frac{1}{q}\right) b(\partial\Lambda^0)$$

Therefore,

$$\beta\tau^0_{1,D}(\Lambda) = -\log \frac{Z^0_{1,D}(\Lambda)}{[Z^0_1(\Lambda)\, Z^0_D(\Lambda)]^{1/2}} = \left[\frac{\beta}{2} + O\left(\frac{1}{q}\right)\right] b(P)$$

because the bonds in the interface are ordered in $Z^0_1(\Lambda)$, but not in $Z^0_{1,D}(\Lambda)$. Thus, the "ground-state energy" of the interface (as $q \to \infty$) is 1/2 (per unit surface), i.e., exactly one-half the ground-state energy of a 1–2 interface.

Now we have to compute low-energy excitations of the interfaces. To be specific, consider $d = 3$. We start with the 1–2 interface: To leading order, we can insert one of the $q-2$ states different from 1 and 2 either into the 1 half-space or into the 2 half-space (see Fig. 3a). This has a weight $e^{-5\beta}$ (for $d = 3$) for the energy times $q-2$ for the entropy, so to leading order, using $\beta_t \approx \frac{1}{3}\log q$, we have

$$\beta_t \tau^E_{12} \approx \beta_t - 2q^{-2/3}$$

The lowest excitations of $Z^E_1(\Lambda)$ are of higher order.

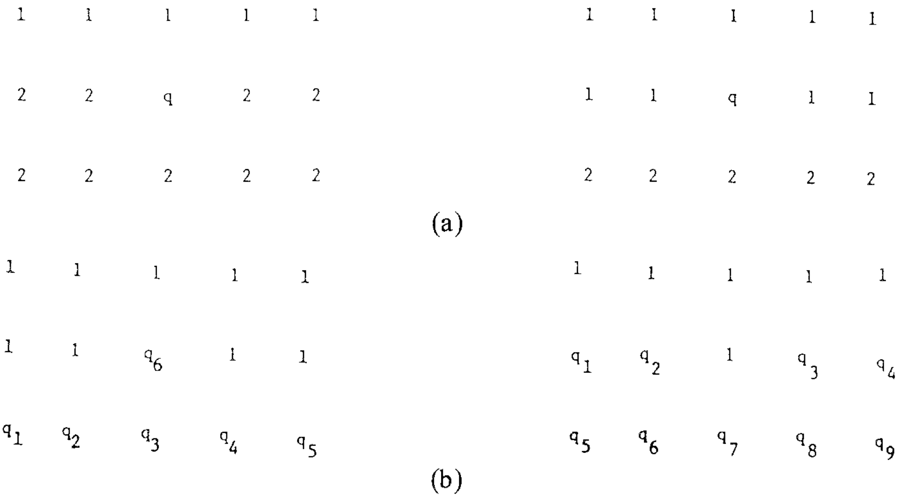


Fig. 3. Lowest energy excitations of the interfaces in the Potts model: (a) 1/2 interface; (b) 1/D interface.

Now we compute τ_{1D}^{E}. We may either insert one spin different from 1 in the ordered half-space (see Fig. 3b), which carries a weight $e^{-5\beta}$ (energy) times q (entropy), or we may insert one spin equal to one in the disordered phase. There one loses q on the entropy side, but gains e^{β} in the energy. However, there is one more term to leading order. As we saw in Section 3.1, the lowest order excitations of the disordered phase have a weight equal to $q^{-2/3}$ (for $\beta_t \approx \frac{1}{3} \log q$). When we compute the restricted surface tension $\tau_{1,D}^{E}$, we have to compare the number of these excitations appearing in $\frac{1}{2} \ln Z_D^E(\Lambda)$ and in $\ln Z_{1,D}^E(\Lambda)$. However, in $Z_{1,D}^E(\Lambda)$ these excitations cannot be located across the interface, while they may occur there in $Z_D^E(\Lambda)$. This adds $\frac{1}{2} q^{-2/3}$ to $\beta \tau_{1D}^E$, where the $\frac{1}{2}$ comes from the $\frac{1}{2}$ multiplying $\ln Z_D^E(\Lambda)$ above (this is similar to the calculation of the "ground-state energy"). The final result for τ_{1D}^E is

$$\beta_t \tau_{1D}^E \approx \tfrac{1}{2}\beta_t - 2q^{-2/3} + \tfrac{1}{2} q^{-2/3} = \tfrac{1}{6} \log q - \tfrac{3}{2} q^{-2/3}$$

and, comparing the two results, we have that in $d=3$, $\beta_t(2\tau_{1D}^E - \tau_{12}^E) \approx -q^{-2/3} < 0$. We therefore expect wetting by the disordered phase at T_t in $d \geqslant 3$. We expect wetting to occur also in $d=2$, but the remarks made at the end of Section 2 can be repeated here. In particular, this model is analogous to the Blume–Capel model with $\gamma = 1$, in the sense that the difference between the restricted surface tensions is produced by low-energy excitations and not by a difference in the "ground-state energies." Numerical simulations were actually done by Selke for $q = 20$,(1) and one sees that the width W_0 of the disordered layer is much smaller than in the Blume–Capel model for $\gamma = 2$.(1,11) W_0 appears to diverge much faster than in the $\gamma = 2$ Blume–Capel model both when the size of the box increases and when the temperatures increases toward T_t. However, the preceding discussion suggests that it may be difficult to find the true asymptotic behavior of this width in feasible numerical simulations, because of the smallness of the free energy difference responsible for its divergence.

It is also quite possible that W_0 appears to diverge faster only because at the temperatures where the numerical simulations are made, one sees only the first few layers of the disordered phase, while the corresponding layers are present at much lower temperatures in the $\gamma = 2$ Blume–Capel model. In any case, we do not see any theoretical reason to expect a different exponent for W_0 in the Potts model than in the $\gamma = 1$ or $\gamma = 2$ Blume–Capel models [i.e., $W_0(T) \approx |T - T_t|^{-1/3}$].

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