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Multilayer Wetting in Clock Models

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We show that the interface between two coexisting phases of the q-state clock model is wetted for any temperature by a stack of films of the phases corresponding to the intermediate angles, assuming q even and $q \geqslant 4$. This follows from the positivity of the spreading coefficients, which we prove using correlation inequalities. A small perturbation of the model exhibits a wetting transition in the low-temperature regime.

KEY WORDS: Multilayer wetting; clock model; correlation inequalities; wetting transitions.

1. INTRODUCTION

We consider the interface between two phases of a system which can have three or more phases in coexistence. Depending on the physical parameters, this interface may be wetted by one or several macroscopic films of the other phases.

This problem has already been studied extensively for three-phase models: in the Blume–Capel model, the interface between the phases "+1" and "−1" is wetted by the "0" phase at the single temperature where the three phases coexist (for fixed values of the other parameters)[1–3] in the three-state chiral clock model one can have a wetted interface above a certain wetting transition temperature.[3,4]

Among the models which have been intensively studied to describe the coexistence of many phases, there are in particular the q-state Potts model ($q \geqslant 4$) and the q-state clock model ($q \geqslant 4$).

The Potts model is completely symmetric: the properties of the interfaces between two ordered phases are the same for any pair of ordered

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phases. Such an interface can therefore only be wetted by the disordered phase. This indeed occurs at the single temperature where all the phases coexist.[1] The case of partially symmetric Potts models has also been considered recently.[5] In this case, interfacial wetting by one or several films also occurs for a discrete set of wetting temperatures.

The present paper is devoted to the clock model where a ground-state analysis shows that interfacial wetting already occurs at $T=0$. Precise definitions will be given in Section 2. Section 3 is devoted to our main result:

$$\tau_{p,p'} \geqslant \tau_{p,p''} + \tau_{p'',p'} \tag{1}$$

for all p, p', p'' with $p<p''<p'$ and $p'-p \leqslant q/2$, and where $\tau_{p,p'}$ is the interfacial tension between the phases corresponding respectively to angles of the clock $2\pi p/q$ and $2\pi p'/q$. Inequality (1) leads directly to

$$\tau_{p,p'} \geqslant \tau_{p,p+1} + \tau_{p+1,p+2} + \cdots + \tau_{p'-1,p'} \tag{2}$$

We thus prove the positivity of a family of spreading coefficients; this implies the Antonov rule

$$\tau_{p,p'} = \tau_{p,p+1} + \tau_{p+1,p+2} + \cdots + \tau_{p'-1,p'}$$

which corresponds to wetting of the p, p' interface by $(p'-p-1)$ films of the intermediate phases.

A small perturbation of the clock model is considered in Section 4. Complete wetting then occurs only above a certain wetting transition temperature.

2. NOTATION

The q-state clock model is defined as follows: at each site $x=(x^1,..., x^d) \in \mathbb{Z}^d$, there is a spin variable $\sigma_x = 0, 1, 2,..., q-1$. Let Λ be a finite box $\subset \mathbb{Z}^d$ which has a section $(2L)^{d-1}$ and a height $2M$,

$$\Lambda = \{x=(x^1,..., x^d) \in \mathbb{Z}^d;\ |x^i| \leqslant L,\ i=1,..., d-1;\ |x^d| \leqslant M\}$$

The Hamiltonian is defined for such a box Λ by

$$\begin{aligned} H_\Lambda\{\sigma_\Lambda, \sigma_{\Lambda^c}\} = &-J \sum_{\substack{\langle x,x'\rangle \\ \in\Lambda}} \cos\frac{2\pi}{q}(\sigma_x - \sigma_{x'}) \\ &-J \sum_{\substack{\langle x,y\rangle \\ x\in\Lambda,\, y\in\Lambda^c}} \cos\frac{2\pi}{q}(\sigma_x - \sigma_y) \end{aligned} \tag{3}$$

where $J \geqslant 0$, $\sum_{\langle x,x' \rangle}$ denotes a sum over nearest neighbors, $\Lambda^c \cup \Lambda = \mathbb{Z}^d$, and σ_Λ, σ_{Λ^c} represent two configurations of spins for Λ and Λ^c, respectively. The conditional Gibbs measure at inverse temperature β is given by

$$\mu_{\Lambda,\beta}(\sigma_\Lambda, \sigma_{\Lambda^c}) = [Z_\Lambda(\beta, \sigma_{\Lambda^c})]^{-1} \exp[-\beta H_\Lambda(\sigma_\Lambda \sigma_{\Lambda^c})]$$

where

$$Z_\Lambda(\beta, \sigma_{\Lambda^c}) = \sum_{\{\sigma_\Lambda\}} \exp[-\beta H_{\Lambda_{L,M}}(\sigma_\Lambda, \sigma_{\Lambda^c})]$$

We now introduce the different possible boundary conditions:

1. The free boundary conditions obtained by omitting the second sum in (3).
2. The ordered p boundary conditions given by $\sigma_y = p$ in the second sum in (3); this leads to the partition function $Z_\Lambda^{p,p}(\beta)$.
3. The mixed (p, p') boundary conditions given by

   $$\sigma_y = p \text{ for } y^d \geqslant 0, \qquad \sigma_y = p' \text{ for } y^d < 0$$

   This leads to the partition function $Z_\Lambda^{p,p'}(\beta)$.

The surface tension between two ordered phases p and p' is then defined as usual by

$$\tau_{p,p'}(\beta) = -\lim_{L \to +\infty} \lim_{M \to +\infty} \left(\frac{1}{2L}\right)^{d-1} \log \frac{Z_\Lambda^{p,p'}(\beta)}{[Z_\Lambda^{p,p}(\beta)]^{1/2} [Z_\Lambda^{p',p'}(\beta)]^{1/2}} \quad (4)$$

3. RESULTS

Due to the symmetries of the model, we can limit ourselves to the cases where $p < p'$ and $p' - p \leqslant q/2$. Let us now state our main results

Theorem. For the q-state clock model defined as above, with q even and $q \geqslant 4$, for $J \geqslant 0$ and any β, one has

$$\tau_{p,p'}(\beta) \geqslant \tau_{p,p''}(\beta) + \tau_{p'',p'}(\beta)$$

for all p, p', p'' such that

$$p < p'' < p' \qquad \text{and} \qquad p' - p \leqslant q/2$$

As a direct consequence of this theorem, we have the following result.

Corollary. For the q-state clock model defined as above with q even and $q \geqslant 4$, for $J \geqslant 0$ and any β, and for all p, p' such that $0 < p' - p \leqslant q/2$, one has

$$\tau_{p,p'}(\beta) \geqslant \tau_{p,p+1}(\beta) + \tau_{p+1,p+2}(\beta) + \cdots + \tau_{p'-1,p'}(\beta)$$

We therefore have a family of spreading coefficients which are positive or zero for any temperature. At equilibrium, spreading coefficients can only be zero or negative. Therefore the corollary should imply the validity of the Antonov rule

$$\tau_{p,p'}(\beta) = \tau_{p,p+1}(\beta) + \tau_{p+1,p+2}(\beta) + \cdots + \tau_{p'-1,p'}(\beta)$$

Of course, this relation makes sense whenever $\tau(\beta) \neq 0$, i.e., when several phases coexist at this temperature β^{-1}. This is known to occur for T small enough in any dimension $d \geqslant 2$.

Proof of the Theorem. Using definition (4) of interfacial tensions, the theorem follows from the following inequality between products of partition functions:

$$Z_{\Lambda}^{p,p'}(\beta)\, Z_{\Lambda}^{p'',p''}(\beta) \leqslant Z_{\Lambda_{L,M}}^{p,p''}(\beta)\, Z_{\Lambda_{L,M}}^{p'',p''}(\beta) \tag{5}$$

which we prove in the following. We have

$$\begin{aligned} &Z_{\Lambda}^{p,p'}(\beta)\, Z_{\Lambda}^{p'',p''}(\beta) \\ &\quad = \sum_{\{\sigma_\Lambda, \sigma'_\Lambda\}} \exp\left\{\beta J \sum_{\substack{\langle x,x'\rangle \\ \in \Lambda}} \left[\cos\frac{2\pi}{q}(\sigma_x - \sigma_{x'}) + \cos\frac{2\pi}{q}(\sigma'_x - \sigma'_{x'})\right]\right. \\ &\qquad \left. + \beta J \sum_{\substack{\langle x,y\rangle \\ x\in\Lambda;\, y\in\Lambda^c}} \left[\cos\frac{2\pi}{q}(\sigma_x - \sigma_y) + \cos\frac{2\pi}{q}(\sigma'_x - \sigma'_y)\right]\right\} \end{aligned} \tag{6}$$

$\sum_{\{\sigma_\Lambda, \sigma'_\Lambda\}}$ is a sum over all pairs of configurations $(\sigma_\Lambda, \sigma'_\Lambda)$ and $\sigma_y = p$, $\sigma'_y = p''$ for the upper part of Λ^c; $\sigma_y = p'$, $\sigma'_y = p''$ for the lower part of Λ^c. The same kind of expression can be written for the rhs of (5).

Let us now consider the measure $\langle \cdot \rangle_0$ induced by (free boundary conditions)

$$H_\Lambda^0(\sigma_\Lambda) = -J \sum_{\substack{\langle x,x'\rangle \\ x\in\Lambda}} \cos\frac{2\pi}{q}(\sigma_x - \sigma_{x'})$$

Dividing both sides of (5) by the square of the partition function associated with H^0, we get

$$a^{p,p''}_{p',p''} \leqslant a^{p,p''}_{p'',p'}$$

where

$$a^{p,p''}_{p',p''} = \left\langle \exp\left\{\beta J \sum_{x\in\partial\Lambda^+} \left[\cos\frac{2\pi}{q}(\sigma_x - p) + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right]\right\} \times \exp\left\{\beta J \sum_{x\in\partial\Lambda^-} \left[\cos\frac{2\pi}{q}(\sigma_x - p') + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right]\right\}\right\rangle_0$$

$$a^{p,p''}_{p'',p'} = \left\langle \exp\left\{\beta J \sum_{x\in\partial\Lambda^+} \left[\cos\frac{2\pi}{q}(\sigma_x - p) + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right]\right\} \times \exp\left\{\beta J \sum_{x\in\partial\Lambda^-} \left[\cos\frac{2\pi}{q}(\sigma_x - p'') + \cos\frac{2\pi}{q}(\sigma'_x - p')\right]\right\}\right\rangle_0$$

where $\partial\Lambda = (x\in\Lambda: d(x, \Lambda^c) = 1\}$, $\partial\Lambda^+$ denotes the upper part of $\partial\Lambda$, and $\partial\Lambda^-$ the lower part. For $p' - p \leqslant q/2$, it remains to show that

$$\left\langle \exp\left\{\beta J \sum_{x\in\partial\Lambda^+} \cos\frac{2\pi}{q}(\sigma_x - p) + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right\} \times \exp\left\{\beta J \sum_{x\in\partial\Lambda^-} \cos\frac{2\pi}{q}(\sigma_x - p') + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right\}\right\rangle_0$$
$$\leqslant \left\langle \exp\left\{\beta J \sum_{x\in\partial\Lambda^+} \cos\frac{2\pi}{q}(\sigma_x - p) + \cos\frac{2\pi}{q}(\sigma'_x - p'')\right\} \times \exp\left\{\beta J \sum_{x\in\partial\Lambda^-} \cos\frac{2\pi}{q}(\sigma_x - p'') + \cos\frac{2\pi}{q}(\sigma'_x - p')\right\}\right\rangle_0 \tag{7}$$

Introducing the Percus variables defined by

$$\alpha_x = \cos\frac{2\pi}{q}\sigma_x + \cos\frac{2\pi}{q}\sigma'_x$$

$$\beta_x = \cos\frac{2\pi}{q}\sigma_x - \cos\frac{2\pi}{q}\sigma'_x$$

$$\gamma_x = \sin\frac{2\pi}{q}\sigma_x + \sin\frac{2\pi}{q}\sigma'_x$$

$$\delta_x = \sin\frac{2\pi}{q}\sigma'_x - \sin\frac{2\pi}{q}\sigma_x$$

we may expand both sides of inequality (7) in powers of βJ. For the rhs, we get a multinomial series in powers of

$$\begin{gathered} \cos\phi_0 \pm \cos\phi_1 \\ \sin\phi_1 \pm \sin\phi_0 \\ \cos\phi_1 \pm \cos\phi_2 \\ \sin\phi_2 \pm \sin\phi_1 \end{gathered}$$

with $\phi_0 = (2\pi/q)\,p$, $\phi_1 = (2\pi/q)\,p''$, $\phi_2 = (2\pi/q)\,p'$. The corresponding coefficients are of the form

$$\langle \alpha^A \beta^B \gamma^C \delta^D \rangle_0 \geqslant 0$$

with

$$\alpha^A = \prod_{x \in A} \alpha_x^{a_x}, \qquad \beta^B = \prod_{x \in B} \beta_x^{b_x}, \qquad \gamma^C = \prod_{x \in C} \gamma_x^{c_x}, \qquad \delta^D = \prod_{x \in D} \delta_x^{d_x}$$

where $a_x, b_x, c_x, d_x \in \mathbb{N}$ and A, B, C, D are subsets of Λ with multiplicity. This positivity can easily be verified provided q is even; the proof is the same as for continuous rotators.[6,7] For the lhs we get the same series except that some coefficients change their sign. This yields inequality (7) whenever all terms in the rhs series are positive. This occurs if we can find p, p'', p' such that

$$\begin{gathered} \cos\phi_0 \geqslant |\cos\phi_1| \\ \sin\phi_1 \geqslant |\sin\phi_0| \\ \cos\phi_1 \geqslant |\cos\phi_2| \\ \sin\phi_2 \geqslant |\sin\phi_1| \end{gathered} \tag{8}$$

Taking into account the rotation invariance of our model, we can choose a reference system with $-\pi/2 \leqslant \phi_0 < 0$ and $\phi_1 = -\phi_0$(see Fig. 1) such that conditions (8) are satisfied, provided $\phi_2 - \phi_0 \leqslant \pi$, or equivalently $p' - p \leqslant q/2$. This completes the proof of (1).

4. PERTURBED CLOCK MODELS

The above theorem is valid at all temperatures and in particular at $T = 0$, where it gives an inequality between ground-state energies under specified boundary conditions. The inequality means that there is a con-

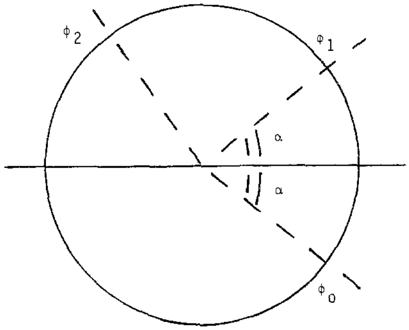

Fig. 1. For a given triple (ϕ_0, ϕ_1, ϕ_2) with $\phi_0 \leqslant \phi_1 \leqslant \phi_2$ and $\phi_2 - \phi_0 \leqslant \pi$, the system of reference is chosen such that the x axis becomes the bisectrix between ϕ_0 and ϕ_1.

figuration with a layer of intermediate angle which has a lower energy than the configurations which are restricted to the two states corresponding to the top and bottom boundary conditions. This means that the inequality (2) does not contradict the Antonov rule

$$\tau_{p,p'}(\beta) = \tau_{p,p+1}(\beta) + \cdots + \tau_{p'-1,p'}(\beta)$$

At $T = 0$, our inequality reduces to

$$\cos\left[\frac{2\pi}{q}(p'-p)\right] + (p'-p) \leqslant (p'-p-1)\cos\left(\frac{2\pi}{q}\right)$$

Whether or not the corresponding equality is verified means that the wetting temperature T_W is zero or does not exist.

Let us now consider a perturbed clock model, which enables one to study the wetting transition. For simplicity, we shall introduce this model in its easiest form, when $q = 4$.

The new Hamiltonian is given by $(J, \varepsilon > 0)$

$$H = \sum_{\langle i,j \rangle} \left(J\left\{1 - \cos\left[\frac{\pi}{2}(\sigma_i - \sigma_j)\right]\right\} + \varepsilon[1 - \cos \pi(\sigma_i - \sigma_j)]\right)$$

To compare a 0–2 interface with 0–1 and 1–2 interfaces, one has to study the corresponding surface tensions. At $T = 0$, it is readily seen that

$$\tau_{02} = 2J$$

$$\tau_{01} = \tau_{12} = J + 2\varepsilon$$

For T small enough it is therefore clear that

$$\tau_{02} < \tau_{01} + \tau_{12}$$

which means that the 0–2 interface is not wetted by a film of "1". However, if one takes into account the first excitations, we get (in dimension $d=2$; the argument works similarly in higher dimension)

$$\tau_{01}=\tau_{12}=J+2\varepsilon-2\beta^{-1}e^{-\beta J}+O(e^{-2\beta J})$$

$$\tau_{02}=2J-2\beta^{-1}e^{-2\beta J}-\frac{4\beta^{-1}e^{-2\beta J-8\beta\varepsilon}}{1-e^{-4\beta\varepsilon}[1+O(e^{-\beta J})]}$$

The last term in τ_{02}, expanded in a geometric series, comes from sums over bubbles of height 1 and length n. The restriction to height 1 in a bubble of length n is an approximation $[1+O(e^{-\beta J})]^n$. Hence the formula. The expansion makes sense only for

$$\varepsilon \ll (1/4\beta)\, O(e^{-\beta J})$$

with the same $O(e^{-\beta J})$, and is seen to diverge when $\varepsilon \uparrow (1/4\beta)\, O(e^{-\beta J})$, where the mean length of bubble diverges. This is not a rigorous result, but we conclude that there must be a wetting transition at some β_W such that

$$\varepsilon \approx \beta_W^{-1} e^{-\beta_W J}$$

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