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Multilayer Wetting in Partially Symmetric q-State Models

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When several phases coexist, the interface between two phases can be wetted by several films of the other phases. This is called *multilayer wetting* and can be characterized by the behavior of the *spreading coefficients*, which relate the surface tensions between the different phases. In this paper we consider a class of models which can exhibit a sequence of phase transitions. With some new correlation inequalities, we prove the positivity of a family of spreading coefficients. These inequalities, together with a thermodynamic argument, lead to the conclusion of multilayer wetting. These results generalize earlier results where single-layer interfacial wetting was obtained for the Potts model.

KEY WORDS: Wetting; multilayer wetting; Potts model; correlation inequalities.

1. INTRODUCTION

When several phases $a_1, a_2, \ldots, a_n$ coexist, an interface between two of them, say a_i, a_{i+2}, may be wetted by a layer of a third one, say a_{i+1}. The condition of perfect wetting of a_i, a_{i+2} by a film of a_{i+1} can be expressed in terms of the spreading coefficient:

$$s(a_i, a_{i+1}, a_{i+2}) = \sigma(a_i, a_{i+2}) - \sigma(a_i, a_{i+1}) - \sigma(a_{i+1}, a_{i+2})$$

where $\sigma(\cdot, \cdot)$ denotes the surface tension between two phases. The interface between the phases a_i, a_{i+2} should be wetted by the phase a_{i+1} when the

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Antonov rule is satisfied: $s(a_i, a_{i+1}, a_{i+2}) = 0$. If all the phases coexist and all the spreading coefficients $s(a_i, a_j, a_k) = 0$ when $i < j < k$, then the interface between the phases a_1 and a_n will be wetted by $n-2$ films of the phases $a_2, \dots, a_{n-1}$. This is *multilayer wetting*. It may be of course that the spreading coefficients define only a partial order between the phases; in such a case, which we shall indeed consider, the number of wetting layers will be smaller.

Among the models which display wetting, of particular interest is the q-state Potts model, whose Hamiltonian is given by

$$H = - \sum_{\langle i,j \rangle} J\delta(\sigma_i, \sigma_j) \tag{1}$$

where $\sigma_i \in \{1, \dots, q\}$, $q \geqslant 2$, $J \geqslant 0$, δ is the usual Kronecker symbol, and the bracket restricts the sum over nearest neighbor pairs. This model exhibits for $d \geqslant 2$ and q not too small a temperature-driven first-order phase transition at some inverse temperature β_t, where q ordered phases $a, b, \dots$ coexist with a disordered phase D; the surface tensions between the coexisting phases are strictly positive; for rigorous results, see refs. 2–6. In ref. 1 some new correlation inequalities were proven and used to prove that the spreading coefficient $s(a, D, b)$ is nonnegative. This result together with a thermodynamic argument led to the conclusion that at β_t the interface between two ordered phases must be wetted by a film of the disordered phase. Actually the correlation inequalities in ref. 1 were proven when q is an even number, and extended to all values of q in ref. 7. A proof that $s(a, D, b) \leqslant 0$ for the Potts model with q large at the transition temperature is given in ref. 8, thus proving the Antonov rule $s(a, D, b) = 0$.

The Antonov rule is compatible only with complete wetting and not with partial wetting; however, in order to describe more precisely this phenomenon, it would be interesting to prove that, indeed, for typical configurations, a macroscopic film of the disordered phase separates the two ordered phases. The thickness of the film is expected to diverge in the thermodynamic limit as $L^{1/2}$ in dimension two and as $\log L$ in dimension three.

In the present paper we give a simpler and more general proof of the correlation inequalities which yield the nonnegativity of spreading coefficients. This proof follows the method of Ginibre[9] as extended to multicomponent rotators.[10,11] It enables us to study multilayer wetting by extending the above analysis to the following class of Hamiltonians:

$$H = - \sum_{\langle i,j \rangle} \sum_{r=1}^{m} J_r \prod_{\alpha=1}^{r} \delta(x_i^\alpha, x_j^\alpha) \tag{2}$$

where

$$x_i^\alpha \in \{1,..., q_\alpha\} \qquad \text{with} \quad \prod_{\alpha=1}^{m} q_\alpha = q$$

so that

$$\sigma = x_i^1 + (x_i^2 - 1)q_1 + (x_i^3 - 1)q_1 q_2 + \cdots + (x_i^m - 1)q_1 \cdots q_{m-1} \tag{3}$$

takes the values 1,..., q.

For $m = 2$, this model exhibits three kinds of pure thermodynamic phases: q ordered phases in which configurations $\{x_i^1\}$ and $\{x_i^2\}$ are both ordered; q_1 partially ordered phases in which only configurations $\{x_i^1\}$ are ordered while $\{x_i^2\}$ are disordered; and a disordered phase in which both configurations are disordered. We expect the phase diagram described in Fig. 2: according to the value of J_2/J_1, either there is a unique inverse transition temperature β_t where the q ordered phases coexist with the disordered one, or there are two transition temperatures β_t^1 and β_t^2 where the partially ordered phases coexist with the ordered ones (β_t^1) or with the disordered one (β_t^2), or for a particular value of J_2/J_1 there is a unique temperature where all the previous phases coexist.

The correlation inequalities mentioned above imply the positivity of spreading coefficients. For example, in the case $m = 2$, consider two ordered phases $a = (a_1, a_2)$, $b = (b_1, b_2)$, two partially ordered phases $a_1 = (a_1$, disordered), $b_1 = (b_1$, disordered), and the totally disordered phase D. We shall prove the following inequalities:

$$\sigma(a, b) \geqslant \sigma(a, D) + \sigma(D, b) \tag{4}$$

$$\sigma(a, b) \geqslant \sigma(a, a_1) + \sigma(a_1, b_1) + \sigma(b_1, b) \tag{5}$$

$$\sigma(a, b) \geqslant \sigma(a, a_1) + \sigma(a_1, D) + \sigma(D, b_1) + \sigma(b_1, b) \tag{6}$$

These results, together with a thermodynamic argument (see ref. 1), lead to wetting by one, two, or three interfacial layers depending on the number of phases in coexistence. For $m > 2$, we obtain similarly up to $2m - 1$ interfacial wetting layers.

2. CORRELATION INEQUALITIES

We first give a simple and general proof of the relevant correlation inequalities for the standard Potts model ($m = 1$). Let Λ be a finite set of sites. To each $i \in \Lambda$ we attach a spin variable σ_i which may assume q values

$\{1, 2,..., q\}$ with $q \geqslant 2$. The energy of a configuration $\sigma_\Lambda \in \{1,..., q\}^{|\Lambda|}$ is given by

$$H(\sigma_\Lambda) = -\sum_{\{i;j\}\subset\Lambda} J_{ij}\,\delta(\sigma_i, \sigma_j) - \sum_{i\in\Lambda} h_i(\sigma_i) \tag{7}$$

We assume that $J_{ij} \geqslant 0$ for all $\{i, j\} \subset \Lambda$. The functions $h_i(\cdot)$ will be used for boundary conditions which will break the symmetry and create an interface. Correlation inequalities involve the fact that the interaction $J_{ij}\,\delta(\sigma_i, \sigma_j)$ is positive definite on $(\mathbb{Z}_q)^\Lambda$. This is not possible for $h_i(\sigma)$ because we shall want to favor one of the q states on the top boundary and a different state on the bottom boundary. In order to retain some symmetry and positive definiteness, we choose an integer k with $1 \leqslant k \leqslant q-1$, and require $h_i(\cdot)$ to be positive definite when restricted to $\mathbb{Z}_k$ and also when restricted to $\mathbb{Z}_{q-k}$:

$$\hat{h}_i'(n) = \frac{1}{k}\sum_{\sigma=1}^{k} h_i(\sigma)\cos\frac{2\pi n\sigma}{k} \geqslant 0 \qquad \text{for all} \quad i\in\Lambda \text{ and } n = 1,..., k \tag{8}$$

and

$$\hat{h}_i''(n) = \frac{1}{q-k}\sum_{\sigma=k+1}^{q} h_i(\sigma)\cos\frac{2\pi n(\sigma-k)}{q-k} \geqslant 0,$$
$$\text{for all} \quad i\in\Lambda \text{ and } n = 1,..., q-k \tag{9}$$

Accordingly, for a given subset $A \subset \Lambda$, let C_k^A denote the set of real, positive-definite functions on the cyclic group $(\mathbb{Z}_k)^A$ (for $k=1$, C_1^A denotes the set of nonnegative functions on A). Let $\mathscr{F}_A$ be the set of real functions of σ_A which vanish unless $\sigma_i \leqslant k$ for all $i\in A$ and whose restriction to $(\mathbb{Z}_k)^A$ belongs to C_k^A. Similarly, let $\mathscr{G}_A$ be the set of real functions of σ_A which vanish unless $\sigma_i \geqslant k+1$ for all $i \in A$ and whose restriction to the remaining subset with the structure of $(\mathbb{Z}_{q-k})^A$ belongs to C_{q-k}^A. We remark that conditions (8) and (9) express that h_i may be written as a sum $h_i^{(1)} + h_i^{(2)}$ where $h_i^{(1)} \in \mathscr{F}_{\{i\}}$ and $h_i^{(2)} \in \mathscr{G}_{\{i\}}$. Let us write

$$\mathscr{F} = \sum_{A\subset\Lambda} \mathscr{F}_A, \qquad \mathscr{G} = \sum_{A\subset\Lambda} \mathscr{G}_A$$

(that is, $\mathscr{F}$ is the set of functions f which may be written as $f = \sum_{A\subset\Lambda} f_A$ with $f_A \in \mathscr{F}_A$ and similarly for $\mathscr{G}$).

Finally let $\langle\cdot\rangle$ denote the expectation value with respect to the Gibbs measure

$$\mu_\Lambda = Z^{-1} e^{-\beta H(\sigma_\Lambda)} \tag{10}$$

Theorem 1. Under the above hypotheses the following inequalities hold:

$$\langle fg\rangle \leqslant \langle f\rangle\langle g\rangle \qquad \text{if} \quad f\in\mathscr{F},\ g\in\mathscr{G} \tag{11}$$

$$\langle f_1 f_2\rangle \geqslant \langle f_1\rangle\langle f_2\rangle \qquad \text{if} \quad f_1, f_2\in\mathscr{F} \tag{12}$$

$$\langle g_1 g_2\rangle \geqslant \langle g_1\rangle\langle g_2\rangle \qquad \text{if} \quad g_1, g_2\in\mathscr{G} \tag{13}$$

Proof. To each $i\in\Lambda$ we attach the angle variables θ_i, ϕ_i, ψ_i belonging, respectively, to $\mathbb{Z}_4$, $\mathbb{Z}_k$, $\mathbb{Z}_{q-k}$, and we make the following change of variables:

If $\sigma_i\leqslant k$, we represent σ_i by $\theta_i=0$ or π, $\phi_i=(2\pi/k)\sigma_i$, and ψ_i arbitrary.
If $\sigma_i\geqslant k+1$, we represent σ_i by $\theta_i=\pi/2$ or $3\pi/2$, $\psi_i=[2\pi/(q-k)]\times(\sigma_i-k)$, and ϕ_i arbitrary.

The Gibbs measure is transformed into

$$\begin{aligned} Z^{-1}\exp\Bigg\{&\sum_{i,j} J_{ij}[\cos^2\theta_i\cos^2\theta_j\,\delta(\phi_i-\phi_j)+\sin^2\theta_i\sin^2\theta_j\,\delta(\psi_i-\psi_j)] \\ &+\sum_i 2\left[\cos^2\theta_i\sum_{n=1}^{k}\hat{h}_i'(n)\cos n\phi_i+\sin^2\theta_i\sum_{n=1}^{q-k}\hat{h}_i''(n)\cos n\psi_i\right] \\ &+\sum_i[\ln(q-k)\cos^2\theta_i+\ln k\sin^2\theta_i]\Bigg\} \end{aligned}$$

where the invariant measure on $\mathbb{Z}_4\times\mathbb{Z}_k\times\mathbb{Z}_{q-k}$ is understood, and where $\delta(\varphi)=1$ if φ is a multiple of 2π and zero otherwise. Therefore μ can be written as

$$Z^{-1}e^{F(\theta_\Lambda,\phi_\Lambda)+G(\theta_\Lambda,\psi_\Lambda)}$$

where $F\in\mathscr{F}$ and $G\in\mathscr{G}$. The proof proceeds now as that of Ginibre inequalities and its generalizations.[9-11] First we introduce the duplicate model with variables $(\theta_i, \phi_i, \psi_i, \theta_i', \phi_i', \psi_i')$ and second we notice that any product of terms of the form

$$(\cos\theta_i\pm\cos\theta_i'),\ (\sin\theta_i'\pm\sin\theta_i)$$

$$\left[\cos\left(\sum m_i\phi_i\right)\pm\cos\left(\sum m_i\phi_i'\right)\right],\ \left[\cos\left(\sum m_i\psi_i'\right)\pm\cos\left(\sum m_i\psi_i\right)\right]$$

(where the m_i are integers) gives a nonnegative contribution when we sum over all values of the variables with respect to the invariant measure. ∎

Remark 1. By choosing $a=k$, $b=q$, and f, g of the form $f=\prod_{i\in A}\delta(\sigma_i, a)$, $g=\prod_{i\in B}\delta(\sigma_i, b)$, where A, B are subsets of Λ, we get the inequalities stated in ref. 1.

Remark 2. The following monotonicity property holds:

$$\langle f\rangle_{(q)}\leqslant\langle f\rangle_{(q-1)} \qquad \text{for all} \quad f\in\mathscr{F} \tag{14}$$

with respect to the number of states ($\mathscr{F}$ being defined with $k=q-1$). In order to see this, we introduce the external field $h_i(\sigma_i)=h\delta(\sigma_i, q)=h\cos^2\theta_i$ and notice that, from Theorem 1, the right-hand side in (14) increases with $h\geqslant 0$, and that for $h=+\infty$ the σ_i will be restricted to the values $\{1,..., q-1\}$.

We next consider a generalized model. Let $q=q_1\cdots q_m$ be the product of m integers $q_r\geqslant 2$ and let the energy be given by

$$H(\sigma_A)=-\sum_{\{i;j\}\subset\Lambda}\sum_{r=0}^{m}J_{ij}(r)\,\delta_{p_r}(\sigma_i, \sigma_j)-\sum_{i\in\Lambda}h_i(\sigma_i) \tag{15}$$

where $p_0=1$, $p_r=q_1\cdots q_r$, and $\delta_p(\sigma, \sigma')=1$ if $\sigma=\sigma'$ modulo p and 0 otherwise. From the correspondence

$$\sigma=x_i^1+(x_i^2-1)\,p_1+(x_i^3-1)\,p_2+\cdots+(x_i^m-1)\,p_{m-1}$$

this Hamiltonian coincides with (2) when $h=0$ and $J_{ij}(r)=J_r$ if i, j are nearest neighbors and zero otherwise. We define

$$D_\sigma^r=\{\sigma'\in\{1,..., q\};\sigma'=\sigma(\mathrm{mod}\ p_r)\}$$

$$n=\frac{q}{p_1}=q_2\cdots q_m$$

and choose some integer k such that $1\leqslant k\leqslant p_1-1$. Now, we say that a real function on σ_A belongs to the set $\mathscr{F}_A$ if it vanishes unless $\sigma_i\in\bigcup_{\sigma=1}^k D_\sigma^1$ for all $i\in A$ and if its restriction to the set $(\bigcup_{\sigma=1}^k D_\sigma^1)^A\cong(\mathbb{Z}_{nk})^A$ belongs to C_{nk}^A. Similarly, we say that a real function on σ_A belongs to the set $\mathscr{G}_A$ if it vanishes unless $\sigma_i\in\bigcup_{\sigma=k+1}^{p_1}D_\sigma^1$ for all $i\in A$ and if its restriction to the set $(\bigcup_{\sigma=k+1}^{p_1}D_\sigma^1)^A\cong(\mathbb{Z}_{n(p_1-k)})^A$ belongs to $C_{n(p_1-k)}^A$. We also assume that $J_{ij}(r)\geqslant 0$ and all $h_i(\cdot)\in\mathscr{F}_{\{i\}}+\mathscr{G}_{\{i\}}$.

Theorem 2. Under these hypotheses, the correlation functions associated with the Hamiltonian (15) satisfy the inequalities stated in Theorem 1.

Proof. As in the proof of Theorem 1, we change σ_i into

$$(\theta_i, \phi_i, \psi_i) \in \mathbb{Z}_4 \times \mathbb{Z}_{nk} \times \mathbb{Z}_{n(p_1-k)}$$

We write $\sigma_i = a_i + r_i p_1$ with $1 \leqslant a_i \leqslant p_1$. Then:

For $a_i \leqslant k$ we take $\theta_i = 0$ or π, $\phi_i = (2\pi/nk)(a_i + r_i k)$, and ψ_i arbitrary.

For $a_i \geqslant k+1$ we take $\theta_i = \pi/2$ or $3\pi/2$, ϕ_i arbitrary, and $\psi_i = [2\pi/n(p_1-k)][a_i - k + r_i(p_1-k)]$.

We have

$$\delta_{p_r}(\sigma_i, \sigma_j) = \cos^2\theta_i \cos^2\theta_j\, \delta\left[\frac{q}{p_r}(\phi_i - \phi_j)\right] + \sin^2\theta_i \sin^2\theta_j\, \delta\left[\frac{q}{p_r}(\psi_i - \psi_j)\right]$$

and we conclude as in the proof of Theorem 1. ∎

3. INEQUALITIES BETWEEN SURFACE TENSIONS

Next, we introduce residual free energies for the class of models defined by (15) which under appropriate conditions (coexistence of the corresponding pure phases) will have the physical meaning of surface tensions or interfacial free energies.[12,13] For this purpose we consider translation-invariant and finite-range interaction potentials and take the set Λ as a rectangular box centered at the origin on a d-dimensional lattice $\mathbb{Z}^d$, and define, for $r = 0, 1,..., m$, the following partition functions with boundary conditions:

$$Z_\Lambda(D_a^r) = \sum_{\sigma_\Lambda;\sigma_{\partial\Lambda}} \exp[-\beta H(\sigma_\Lambda \mid \sigma_{\partial\Lambda})] \prod_{i\in\partial\Lambda} \left(\frac{p_r}{q}\right) \delta_{p_r}(\sigma_i, a) \tag{16}$$

where $\partial\Lambda$ denotes the boundary of Λ (with a thickness equal to the range of the interaction) and

$$H(\sigma_\Lambda \mid \sigma_{\partial\Lambda}) = H(\sigma_{\Lambda\cup\partial\Lambda}) - H(\sigma_{\partial\Lambda})$$

In particular, the case $r = m$ corresponds to totally ordered boundary conditions, and $r = 0$ corresponds to free boundary conditions. We also introduce mixed boundary conditions $(D_a^r, D_b^{r'})$ with respect to a plane containing the origin, orthogonal to a d-dimensional vector $\mathbf{n}$, and the corresponding partition functions

$$Z_\Lambda(D_a^r \mid D_b^{r'}) = \sum_{\sigma_\Lambda;\sigma_{\partial\Lambda}} \exp[-\beta H(\sigma_\Lambda \mid \sigma_{\partial\Lambda})] \prod_{i\in\partial\Lambda^+} \left(\frac{p_r}{q}\right) \delta_{p_r}(\sigma_i, a) \times \prod_{i\in\partial\Lambda^-} \left(\frac{p_{r'}}{q}\right) \delta_{p_{r'}}(\sigma_i, b)$$

where $\partial\Lambda^+$ is the part of $\partial\Lambda$ located above the plane and $\partial\Lambda^- = \partial\Lambda \backslash \partial\Lambda^+$. We define the surface tension at inverse temperature β by

$$\sigma^{\mathbf{n}}(D_a^r, D_b^{r'}) = \lim_{\Lambda \uparrow \mathbb{Z}^d} -\frac{1}{\beta S_\Lambda(\mathbf{n})} \log \frac{Z_\Lambda(D_a^r, D_b^{r'})}{[Z_\Lambda(D_a^r)\, Z_\Lambda(D_b^{r'})]^{1/2}} \tag{17}$$

where $S_\Lambda(\mathbf{n})$ is the area of the portion of the plane orthogonal to $\mathbf{n}$ inside Λ.

Theorem 3. If $r' \leqslant r$ and $a \neq b \pmod{p_1}$, we have

$$\sigma^{\mathbf{n}}(D_a^r, D_b^r) \geqslant \sigma^{\mathbf{n}}(D_a^r, D_a^{r'}) + \sigma^{\mathbf{n}}(D_a^{r'}, D_b^{r'}) + \sigma^{\mathbf{n}}(D_b^{r'}, D_b^r) \tag{18}$$

$$\sigma^{\mathbf{n}}(D_a^r, D_b^{r''}) \geqslant \sigma^{\mathbf{n}}(D_a^r, D_a^{r'}) + \sigma^{\mathbf{n}}(D_a^{r'}, D_b^{r''}) \qquad \forall r'' \tag{19}$$

Proof. Let us begin with (18), which in finite volume is equivalent to

$$\frac{Z_\Lambda(D_a^r, D_b^r)}{Z_\Lambda(D_a^r)^{1/2}\, Z_\Lambda(D_b^r)^{1/2}} \leqslant \frac{Z_\Lambda(D_a^r, D_a^{r'})}{Z_\Lambda(D_a^r)^{1/2}\, Z_\Lambda(D_a^{r'})^{1/2}} \frac{Z_\Lambda(D_a^{r'}, D_b^{r'})}{Z_\Lambda(D_a^{r'})^{1/2}\, Z_\Lambda(D_b^{r'})^{1/2}} \frac{Z_\Lambda(D_b^{r'}, D_b^r)}{Z_\Lambda(D_b^{r'})^{1/2}\, Z_\Lambda(D_b^r)^{1/2}}$$

or

$$\frac{Z_\Lambda(D_a^r, D_b^r)}{Z_\Lambda(D_a^{r'}, D_b^{r'})} \leqslant \frac{Z_\Lambda(D_a^r, D_a^{r'})}{Z_\Lambda(D_a^{r'})} \frac{Z_\Lambda(D_b^{r'}, D_b^r)}{Z_\Lambda(D_b^{r'})} \tag{20}$$

This last inequality follows by a chain of inequalities: let $\langle \cdot \rangle_{a,r;b,r'}$ denote the expectation in the ensemble $(D_a^r, D_b^{r'})$. We first use (11) to obtain ($r' \leqslant r$ is necessary here)

$$\left\langle \prod_{i \in \partial\Lambda^+} \delta_{p_r}(\sigma_i, a) \prod_{i \in \partial\Lambda^-} \delta_{p_r}(\sigma_i, b) \right\rangle_{a,r';b,r'} \leqslant \left\langle \prod_{i \in \partial\Lambda^+} \delta_{p_r}(\sigma_i, a) \right\rangle_{a,r';b,r'} \left\langle \prod_{i \in \partial\Lambda^-} \delta_{p_r}(\sigma_i, b) \right\rangle_{a,r';b,r'} \tag{21}$$

We then use (12) to prove

$$\left\langle \prod_{i \in \partial\Lambda^+} \delta_{p_r}(\sigma_i, a) \right\rangle_{a,r';b,r'} \leqslant \left\langle \prod_{i \in \partial\Lambda^+} \delta_{p_r}(\sigma_i, a) \right\rangle_{a,r';a,r'} \tag{22}$$

and (13) to prove

$$\left\langle \prod_{i \in \partial\Lambda^-} \delta_{p_r}(\sigma_i, b) \right\rangle_{a,r';b,r'} \leqslant \left\langle \prod_{i \in \partial\Lambda^-} \delta_{p_r}(\sigma_i, b) \right\rangle_{b,r';b,r'} \tag{23}$$

Combining (21)–(23) gives (20), which proves (18). One could be worried that we have omitted factors of the kind (p_r/q) which were present in (16); it can be checked that they factor out in the above argument. We now turn to (19), which in finite volume is equivalent to

$$\frac{Z_A(D_a^r, D_b^{r''})}{Z_A(D_a^r)^{1/2}\, Z_A(D_b^{r''})^{1/2}} \leqslant \frac{Z_A(D_a^r, D_a^{r'})}{Z_A(D_a^r)^{1/2}\, Z_A(D_a^{r'})^{1/2}} \frac{Z_A(D_a^{r'}, D_b^{r''})}{Z_A(D_a^{r'})^{1/2}\, Z_A(D_b^{r''})^{1/2}}$$

or

$$\frac{Z_A(D_a^r, D_b^{r''})}{Z_A(D_a^{r'})} \leqslant \frac{Z_A(D_a^r, D_a^{r'})}{Z_A(D_a^{r'})} \frac{Z_A(D_a^{r'}, D_b^{r''})}{Z_A(D_a^{r'})} \tag{24}$$

or

$$\left\langle \prod_{i \in \partial A^+} \delta_{p_r}(\sigma_i, a) \prod_{i \in \partial A^-} \delta_{p_{r''}}(\sigma_i, b) \right\rangle_{a, r'; a, r'}$$
$$\leqslant \left\langle \prod_{i \in \partial A^+} \delta_{p_r}(\sigma_i, a) \right\rangle_{a, r', a, r'} \left\langle \prod_{i \in \partial A^-} \delta_{p_{r''}}(\sigma_i, b) \right\rangle_{a, r'; a, r'} \tag{25}$$

which is of the form (11) provided $r' \leqslant r$. This concludes the proof of Theorem 3. ∎

Theorem 3 can be used iteratively; e.g., we have the following result.

Corollary.

$$\sigma(a, b) \geqslant \sigma(a, D_a^{m-1}) + \sigma(D_a^{m-1}, D_a^{m-2}) + \cdots + \sigma(D_a^1, D) + \sigma(D, D_b^1)$$
$$+ \cdots + \sigma(D_b^{m-2}, D_b^{m-1}) + \sigma(D_b^{m-1}, b)$$

4. DISCUSSION

We first consider the Hamiltonian (2) for $m = 2$:

$$H(\sigma_A) = -\sum_{\langle i, j \rangle \subset A} J_1\, \delta(x_i^1, x_j^1) + J_2\, \delta(x_i^1, x_j^1)\, \delta(x_i^2, x_j^2)$$
$$= -\sum_{\langle i, j \rangle \subset A} J_1\, \delta_{q_1}(\sigma_i, \sigma_j) + J_2\, \delta(\sigma_i, \sigma_j) \tag{26}$$

and give a brief discussion about the phase diagram associated with this model. Let us consider the following restricted ensembles[4]:

1. The q ordered restricted ensembles which are the states supported by a single configuration where all the spins are identical, i.e., $\sigma_i = a$ for $a = 1, 2, \ldots, q$.

2. The partially ordered ensembles where all $\sigma_i \in D_a^1$ with equidistributed probability on these configurations. When $a = 1, \ldots, q$ there are q_2 different partially ordered restricted ensembles.

3. The disordered restricted ensemble denoted by D which gives equal probability to all configurations.

Taking into account the energy and the entropy contributions associated with these sets of configurations, we see that the weights of the restricted ensembles are proportional to $\exp[\beta(J_1 + J_2)\, l(\Lambda)]$ in case 1, to $\exp[\beta J_1\, l(\Lambda) + |\Lambda| \ln q_2]$ in case 2, and to $\exp(|\Lambda| \ln q)$ in case 3, where $l(\Lambda)$ is the number of nearest neighor pairs inside Λ and $|\Lambda|$ is the number of sites. At the point $P = ((1/d) \ln q_1, (1/d) \ln q_2)$ in the plane $\beta J_1, \beta J_2$ the three weights are equal. There are three straight lines starting form P where two of the weights coincide. These lines divide the plane $\beta J_1, \beta J_2$ in three regions (1), (2), and (3), where one of the weights is dominant (see Fig. 1).

Such restricted ensembles appear as the limit of the equilibrium states of the system when q_1, q_2, and β tend to infinity. Therefore, to each restricted ensemble a pure thermodynamic phase can be associated, and the phase diagram for large q_1 and q_2 should mimic the above structure as shown in Fig. 2. A proof of it might be obtained either by using the generalization of the Pirogov–Sinai theory theory proposed in ref. 4 or by extending the method of ref. 6.

A proof of the existence of these different pure phases, which gives a partial description of the phase diagram, can already be obtained by means

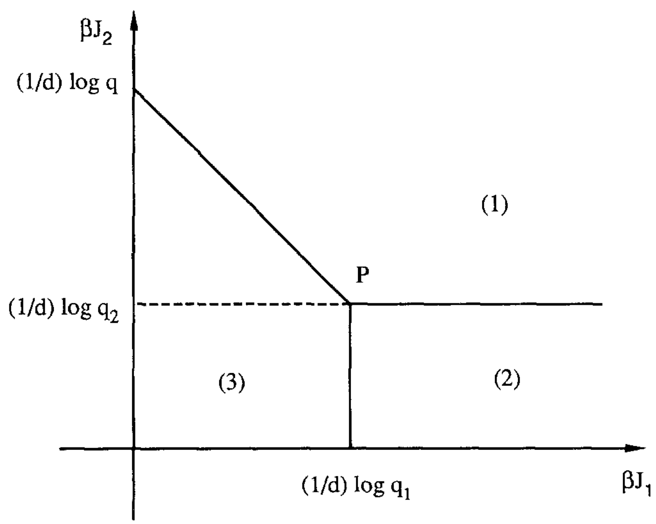

Fig. 1. Diagram of restricted ensembles.

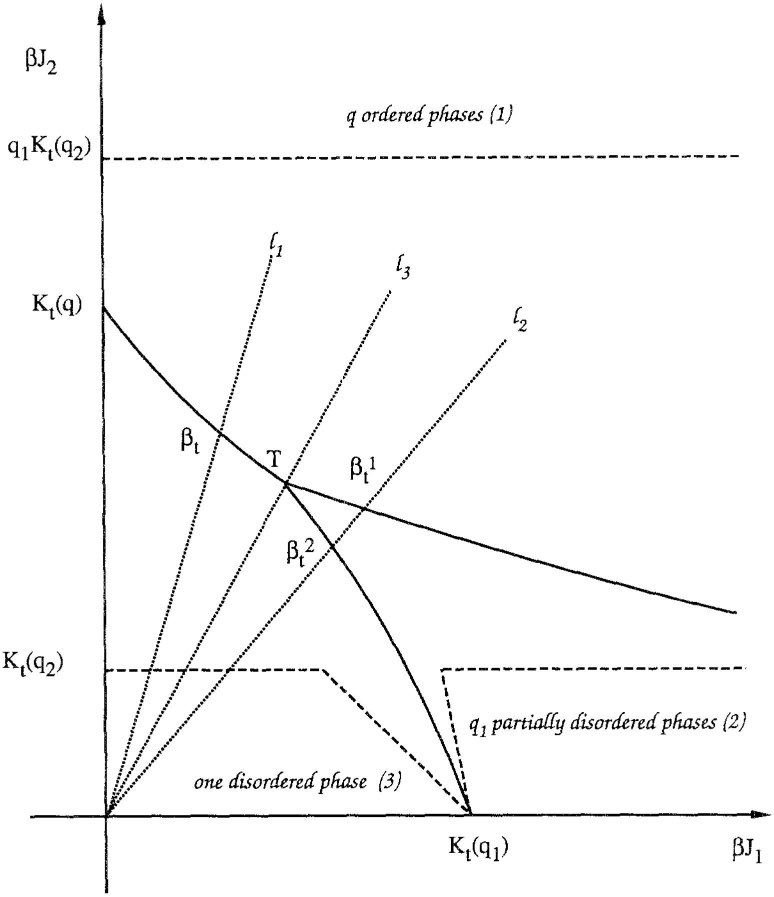

Fig. 2. Expected phase diagram for Hamiltonian (26).

of correlation inequalities. This proof is valid for any value of q_1 and q_2 provided the usual Potts models with these numbers of states have a first-order transition. We let $a = a_1 + (a_2 - 1)q_1$, $a_i \in \{1,..., q_i\}$, and denote by $\langle \cdot \rangle_A^a(J_1, J_2)$ the expectation value with respect to the measure (10) under the ordered boundary condition "a":

$$\langle \cdot \rangle_A^a(J_1, J_2) = Z_A^{-1}(a) \sum_{\sigma_A;\sigma_{\partial A}} \exp[-\beta H(\sigma_A \mid \sigma_{\partial A})] \prod_{i \in \partial A} \delta(\sigma_i, a) \tag{27}$$

and denote by $\langle \cdot \rangle^a(J_1, J_2)$ the corresponding thermodynamic limit. We let $K_t(q)$ denote the value of the coupling constant at the transition point for the q-state, d-dimensional Potts model and introduce the order parameters

$$m_1 = \langle q_1\, \delta(x_i^1, a_1) - 1) \rangle^a(J_1, J_2) \tag{28}$$

$$m_2 = \langle q_2\, \delta(x_i^2, a_2) - 1 \rangle^a(J_1, J_2) \tag{29}$$

Theorem 4. Under the above hypothesis we have:

1. If $\beta J_1 + \beta J_2/q_2 \geqslant K_t(q_1)$ and $\beta J_2/q_1 \geqslant K_t(q_2)$, then $m_1 > 0$ and $m_2 > 0$.
2. If $\beta J_1 + \beta J_2/q_2 \geqslant K_t(q_1)$ and $\beta J_2 < K_t(q_2)$, then $m_1 > 0$ and $m_2 = 0$.
3. If $\beta J_1 + \beta J_2 < K_t(q_1)$ and $\beta J_2 < K_t(q_2)$, then $m_1 = 0$ and $m_2 = 0$.

Proof. We adapt to our case the method of ref. 14. We here use the fact that $q_\alpha\,\delta(x_i^\alpha, x_j^\alpha) - 1$ can be written as a sum of cosines and apply Ginibre inequalities.[9] Then

$$0 \leqslant \langle q_2\,\delta(x_i^2, a_2) - 1\rangle_\Lambda^a (J_1, J_2)$$
$$\leqslant \langle q_2\,\delta(x_i^2, a_2) - 1\rangle_\Lambda^a (J_1 = \infty, J_2) = M_{\Lambda, q_2}(J_2)$$

where $M_{\Lambda,q}(J)$ denotes the magnetization of the q-state Potts model, i.e.,

$$M_{\Lambda,q}(J) = \langle q\delta(x_i^1, a_1)\,\delta(x_i^2, a_2) - 1\rangle_\Lambda^a (0, J)$$

We add to the Hamiltonian the term $\lambda \sum_{\langle i,j\rangle} \delta(x_i^2, x_j^2)$. The expectation of $q_2\,\delta(x_i^2, a_2) - 1$ for $\lambda = 0$ is less than the same expectation for $\lambda = \infty$, and therefore

$$0 \leqslant \langle q_1\,\delta(x_i^1, a_1) - 1\rangle_\Lambda^a (J_1, J_2) \leqslant M_{\Lambda, q_2}(J_1 + J_2)$$

Finally we notice that each term of the sum in the Hamiltonian can be written as

$$J_1\,\delta(x_i^1, x_j^1) + J_2\left(\delta(x_i^1, x_j^1) - \frac{1}{q_1}\right)\left[\delta(x_i^2, x_j^2) - \frac{1}{q_2}\right]$$
$$+ \frac{J_2}{q_2}\,\delta(x_i^1, x_j^1) + \frac{J_2}{q_1}\,\delta(x_i^2, x_j^2) - \frac{J_2}{q}$$

and we get

$$\langle q_1\,\delta(x_i^1, a_1) - 1)\rangle_\Lambda^a (J_1, J_2) \geqslant M_{\Lambda, q_1}\left(J_1 + \frac{J_2}{q_2}\right)$$

$$\langle q_2\,\delta(x_i^2, a_2) - 1\rangle_\Lambda^a (J_1, J_2) \geqslant M_{\Lambda, q_2}\left(\frac{J_2}{q_1}\right)$$

The proof of the theorem then follows from the fact that $M_q(J) > 0$ if $\beta J \geqslant K_t(q)$ and zero otherwise. ∎

The regions where Theorem 4 applies are shown in Fig. 2 (see dashed lines), which has been drawn in the case $q_1 \geqslant q_2$. The case $q_1 < q_2$ is analogous.

Immediate consequences of Theorem 3 are inequalities (4)–(6) stated in the Introduction as well as

$$\begin{aligned} \sigma(a, b_1) &\geqslant \sigma(a, a_1) + \sigma(a_1, b_1) \\ \sigma(a, D) &\geqslant \sigma(a, a_1) + \sigma(a_1, D) \\ \sigma(a_1, b_1) &\geqslant \sigma(a_1, D) + \sigma(D, b_1) \end{aligned} \tag{30}$$

where a_1, b_1, and D coincide, respectively, with $D^1_{a_1}$, $D^1_{b_1}$, and D^0_b (for any b). Taking into account the expected phase diagram of Fig. 2, we see that three different behaviors of our system are possible when the temperature varies. They correspond to the three cases described in the Introduction and occur, as shown in Fig. 2 (lines l_1, l_2, l_3), according to wether J_2/J_1 is larger than, less than, or equal to its value at the triple point T. Inequalities (4)–(6) and (30) then lead to the following conclusions: In the first case at the transition inverse temperature β_t, where the ordered and the disordered phases coexist, two different ordered phases a, b are wetted by a layer of the disordered phase D. Similarly, in the second case at β_t^2, where the partially ordered and the disordered phases coexist, a layer of the disordered phase D wets two partially ordered phases a_1, b_1. On the other hand, at β_t^1, where the ordered and the partially ordered phases coexist, the interface $a|b$ is wetted by the two layers of phases a_1 and b_1. Also the interface, $a|b_1$ is wetted by a layer of phase a_1. In the third case, at the transition point where all different phases coexist, it appears that the interface $a|b$ is wetted by the three layers of phases a_1, D, and b_1, etc.

We finally consider the general Hamiltonian (2). In this case we expect, together with the q ordered and one disordered phase, $m-1$ kinds of partially ordered phases. They are associated with the partially ordered restricted ensembles of type r, for $r = 1,..., m-1$, which have their support on the set of configurations such that $\sigma_i \in D^r_a$ for all i. When $a = 1,..., q$ this leads to p_r different states of type r. According to the values of the interactions J_r several first-order transitions may occur. At these transition points, the inequalities of Theorem 3 and their consequences suggest multilayer wetting phenomena, the wetting layers of the coexisting phases being placed according to the partial order between pure phases defined by their type r.

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