Bond percolation problem in a semi-infinite medium. Landau-Ginzburg theory

Alba Theumann

Department of Physics, Polytechnic Institute of New York, 333 Jay Street, Brooklyn, New York 11201
(Received 26 September 1978)

The bond percolation problem in a lattice bound by a plane surface is defined by associating different occupation probabilities P_B, $P_\parallel$, or $P_\perp$ to bonds in the bulk, on the surface, or linking the bulk to the surface, respectively. The coordinate z indicates the distance of parallel planes to the surface. The z-dependent percolation probability $\varphi(z)$ is defined as the probability that a site on the plane z belongs to an infinite cluster and I derive a rigorous expression for $\varphi(z)$ by introducing z-dependent external fields h_z in the q states Potts Hamiltonian in the limit $q = 1$. Gaussian integration techniques are used to derive a Landau-Ginzburg free-energy functional for arbitrary q. The resulting differential equations for the order parameter are explicitly solved for the bond percolation problem. We introduce the parameters $t = 2n \ln[q_B/q_c]$ and $\omega = 2\ln[q_\parallel^{n_s} q_\perp/q_c^n]$, where $q_\alpha = 1 - P_\alpha$ is the probability of a bond being absent, and $n(n_s)$ is the coordination number in the bulk (surface). Also $P_c = 1 - \exp(-1/n)$ is the mean-field value of the percolation concentration of bonds in the bulk. We obtain the following results: (a) for $t > 0$, $\omega_s < \omega < t$, where $\omega_s = -1/2(t/n)^{1/2}$, all clusters are finite; (b) for $t > 0$, $\omega < \omega_s$, all clusters are finite in the bulk but the probability for an infinite cluster to form at and near the surface is nonvanishing; (c) for $\omega < t < 0$ an infinite cluster forms through the whole system, but it has a larger probability of being close to the surface; (d) for $0 < t < \omega$ only finite clusters occur in the system; (e) for $\omega > t$ and $t < 0$, an infinite cluster starts to form in the whole system, with a larger probability of being in the bulk than on the surface. Critical exponents are derived for the different transitions and they are shown to satisfy general scaling relations.

I. INTRODUCTION

In the bond percolation model, bonds connecting nearest-neighbor sites of an infinite lattice can be present (or absent) at random with probability p (or $1-p$). The occupied bonds form clusters, and for $p < p_c$ all clusters are finite, while for $p > p_c$ an infinite cluster starts to form. One physical quantity of interest here is the percolation probability φ of the lattice, that is, the probability that a site belongs to an infinite cluster. The percolation probability plays the role of the order parameter in this problem, it is nonvanishing only for $p > p_c$ and equal to unity for $p = 1$.

The percolation transition has been studied by Dunn *et al.*[1] and Essam *et al.*[2] by considering the dilute Ising model with nearest-neighbor interactions in the "percolation limit" $T \to 0$ where T is the absolute temperature. The bond percolation model can also be formulated as the limit $q = 1$ of the q-states Potts model.[3,4] The relationship between Potts and bond percolation models has been first discussed by Fortuin and Kasteleyn.[5]

The problem I investigate here is bond percolation in a semi-infinite lattice with a plane surface. I consider for simplicity a simple cubic lattice and the surface to be a $(0, 0, 1)$ plane.

Bonds on the surface and linking the surface to the bulk are considered to have, in general,

different occupation probabilities that differ also from the bulk occupation probability. A given bond can then be present with a probability $p_\parallel$, $p_\perp$, or p_B if it connects two sites on the surface, one site on the surface and one in the bulk, or two sites in the bulk, respectively. Planes parallel to the surface are labeled by the coordinate $z > 0$, while the surface is at $z = 0$.

By generalizing standard definitions in percolation theory,[1-5] we define the z-dependent percolation probability $\varphi(z)$ as the probability that a site on the z plane belongs to an infinite cluster.

In Sec. II, I follow closely the method of Ref. 3 and generalize it by the introduction of z-dependent fields h_z in the q-states Potts model. An effective free energy $F(\{h\})$ is defined by taking the appropriate limit $q = 1$, and we establish the formal relationship between $\varphi(z)$ and the partial derivative of $F(\{h\})$ with respect to h_z, in zero field. In Sec. III, I use Gaussian integration techniques to derive the Landau-Ginzburg free-energy functional,[6] in the continuum limit, for the q-states Potts model. In Sec. IV the differential equations for the order parameter, obtained by functional differentiation of the free energy, are analyzed for all values of q. The analytical solutions of these equations becomes difficult for $q \geqslant 3$, because in this case the Potts model has a discontinuous transition,[7,8] and the jump in the order parameter from zero to a finite value prevents a perturbation expansion. For $q = 2$, the Potts model cor-

responds to the Ising model,[5] and this problem
has been widely investigated within the context
of Landau–Ginzburg theory.[9]

   The percolation transition, described by the
appropriate limit $q = 1$, is again continuous. Close
to the transition, the free-energy functional can
be truncated by keeping only the third and second
power of the order parameter in the bulk and
surface terms, respectively. The differential
equations obtained in this way are easily inte-
grated with the following results: analogous to the
Ising case[6,9] we can identify an inverse extrapola-
tion length or "surface force" λ^{-1} that depends on
the bulk and surface occupation probabilities.
I introduce the parameters $t = 2n \ln[q_B/q_c]$ and
$\omega = 2 \ln(q_{\parallel}^{n_s} q_{\perp}/q_c^n)$ where n and n_s are the number
of nearest neighbors in the bulk and on the sur-
face, respectively, and $q_\alpha = 1 - p_\alpha$ is the probabil-
ity of a bond being absent. Here $q_c = 1 - p_c$ is the
percolation concentration of vacancies in the bulk
and $\ln[q_c^{-1}] = n^{-1}$ in mean-field theory.[3] The sign
of λ^{-1} is determined by the sign of $\omega - t$ and we
can identify four different cases: (a) When $\lambda^{-1} > 0$
and $t > 0$, all clusters are finite; (b) for $\lambda^{-1} > 0$
and $t < 0$ an infinite cluster starts to form with a
larger probability of being in the bulk that on the
surface; (c) when $\lambda^{-1} < 0$ and $t > 0$ the bulk has
too many vacancies for an infinite cluster to ap-
pear, but an infinite cluster may form in the
neighborhood of the surface for sufficiently large
values of $p_{\parallel}, p_{\perp}$. The condition for this surface
cluster to exist is that $\omega < \omega_S(t)$, where $\omega_S(t)$
$= -\frac{1}{2}(t/n)^{1/2}$; (d) when $\lambda^{-1} < 0$ and $t < 0$ the infinite
cluster extends to the bulk, but it keeps a larger
probability of being close to the surface. These
transitions can be identified with the surface,
ordinary, and extraordinary transitions defined
by Lubensky and Rubin,[9] and the corresponding
critical exponents are given at the end of Sec.
IV. The exponents for the ordinary transition are
shown to satisfy the scaling relations of Bray
and Moore.[10]

II. GENERAL RELATIONS

   In the q-states Potts model every site of a
lattice is occupied by a spin $\sigma_{\vec{R}}$ which can take on
q different values. Nearest-neighbor spins have
an interaction energy $-\epsilon$ if they are in the same
state and 0 otherwise. When the Potts model is
used to describe the percolation problem, the
interaction energy $-\epsilon$ is related to the bond oc-
cupation probability.[3] To treat the percolation
problem in a semi-infinite medium we consider
then the interaction energy to be $\epsilon_{\parallel}$, $\epsilon_{\perp}$, or ϵ_B
if the two spins are on the surface, one on the
surface and the other in the bulk, or both in the

bulk, respectively. We consider a lattice with L
planes and M sites by plane. Sites are labeled
by the coordinate $\vec{R} = (\vec{r}, z)$, where $\vec{r}$ indicates the
position on a plane, $0 \le z \le L$ and the surface is at
$z = 0$. The Hamiltonian is then:

$$-\beta \mathcal{H} = \frac{1}{2} \sum_{(\vec{R}, \vec{R}')} K(\vec{R}, \vec{R}') \delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'})$$

$$+ \sum_{\vec{R}} h_z \delta[\sigma_{\vec{R}} - 1] \qquad (2.1)$$

where we introduced z-dependent external fields
coupled to one of the components of $\sigma_{\vec{R}}$. The
first sum runs only over nearest-neighbor pairs
and

$$K(\vec{R}, \vec{R}') = \begin{cases} K_B = \beta\epsilon_B & \text{if } z, z' > 0 \\ K_\perp = \beta\epsilon_\perp & \text{if } z(z') = 0, z'(z) > 0 \\ K_{\parallel} = \beta\epsilon_{\parallel} & \text{if } z = z' = 0 \\ 0 & \text{otherwise.} \end{cases} \qquad (2.2)$$

The partition function is then

$$Q = \mathrm{Tr}\{\sigma\} \prod_{(\vec{R}, \vec{R}')} [1 + v(\vec{R}, \vec{R}')\delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'})]$$

$$\times \exp\left(\sum_{\vec{R}} h_z \delta(\sigma_{\vec{R}} - 1) \right), \qquad (2.3)$$

where $v(\vec{R}, \vec{R}') = e^{K(\vec{R}, \vec{R}')} - 1$. Stephen (Ref. 3,
Appendix A) showed that the trace can be evalu-
ated by expanding the product in Eq. (2.3) and
by assigning a weight 1 to an "empty" bond and
a weight $v(\vec{R}, \vec{R}')$ to an "occupied" bond. In this
way the product over nearest neighbors splits
into a sum over "graphs" or configurations G,
where every graph is a given distribution of bonds
in the lattice.[5] Lattice sites fall into clusters,
and due to the $\delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'})$ term in Eq. (2.3), all
sites in a connected cluster $C(G)$ are in the same
state σ_c. The smallest connected cluster has a
single site and for the moment we consider a
large but finite lattice of L planes and M sites
per plane. Following the same steps as in Ref. 3
we obtain

$$Q = \sum_G v_B^{\eta_B(G)} v_\perp^{\eta_\perp(G)} v_{\parallel}^{\eta_{\parallel}(G)}$$

$$\times \prod_{C(G)} \left[\exp\left(\sum_{z \in C} h_z \xi_z(C) \right) + (q - 1) \right], \qquad (2.4)$$

where $v_\alpha = e^{K_\alpha} - 1$, $\alpha = B$, $\parallel$, or $\perp$ from Eq. (2.2).
Here $\eta_\alpha(G)$ indicates, for a given graph G, the
total number of occupied bonds in the bulk, sur-
face, or perpendicular to the surface if $\alpha = B$,
$\parallel$, or $\perp$, respectively. The product in Eq. (2.4)
is over all connected clusters $C(G)$ of a given

graph G and

$$\xi_z(C) = N_{C(G)} \tag{2.5}$$

where $N_{C(G)}$ is the number of sites in the cluster $C(G)$ that are on the plane z. It is obvious that $\sum_{z=0}^{L} \xi_z(C)$ is the total number of sites of cluster C, and for $K_{\parallel} = K_{\perp} = K_B$ and constant field Eq. (2.4) reduces to Eq. (A3) of Ref. 3. In the same way, the correct description of the bond percolation model is obtained if we associate the weight

$$v_\alpha = e^{K_\alpha} - 1 = p_\alpha/(1 - p_\alpha), \quad \alpha = B, \parallel, \text{ or } \perp, \tag{2.6}$$

where p_B, $p_{\parallel}$, or $p_{\perp}$ are the occupation probabilities for a bond in the bulk, on the surface, or linking the surface to the bulk, respectively.

We find it convenient to define the free energy per surface site:

$$F(\{h\}) = -\frac{1}{M}\left(\frac{\partial}{\partial q}\ln Q\right)_{q=1}$$

$$= -\frac{1}{M}\sum_G W(G)\sum_{C(G)}\exp\left(-\sum_{z \in C} h_z \xi_z(C)\right) \tag{2.7}$$

where

$$W(G) = \prod_\alpha \left[v_\alpha^{\eta_\alpha(G)}(1 + v_\alpha)^{-\eta_\alpha}\right]$$

is the probability of occurrence of the graph G. Here η_α indicates the total number of bonds in the bulk, surface, or perpendicular to the surface for $\alpha = B, \parallel,$ or $\perp$, and only finite clusters contribute to the sum in Eq. (2.7).

We call

$$M\gamma(\xi_0, \ldots, \xi_L; G) \tag{2.8}$$

the number of finite clusters in G with ξ_0 sites on $z = 0$; ξ_L sites on $z = L$, and we can then write from Eq. (2.7)

$$F(\{h\}) = -\sum_{\xi_0=1}^{M}\cdots\sum_{\xi_L=1}^{M}\gamma(\xi_0, \ldots, \xi_L)$$

$$\times \exp\left(-\sum_{z=0}^{L} h_z \xi_z\right), \tag{2.9}$$

where

$$\gamma(\xi_0, \ldots, \xi_L) = \sum_G W(G)\gamma(\xi_0, \ldots, \xi_L; G) \tag{2.10}$$

is the average number of finite clusters with ξ_0 sites on $z = 0$; ξ_L sites on $z = L$.

We obtain for the partial derivative of $F(\{h\})$ with respect to h_z in zero field

$$W_z = \left(\frac{\partial}{\partial h_z}F(\{h\})\right)_{h=0} = \sum_{\xi=1}^{M}\xi\gamma_z(\xi) = \sum_{\xi=1}^{M} W_z(\xi) \tag{2.11}$$

where

$$\gamma_z(\xi_z) = \sum_{\text{all }\xi \neq \xi_z} \gamma(\xi_0, \ldots \xi_z, \ldots, \xi_L)$$

is the average number of finite clusters with ξ_z sites on the plane z. Hence we conclude that $W_z(\xi) = \xi\gamma_z(\xi)$ is the probability that a site on z belongs to a finite cluster with ξ sites on the plane z. W_z in Eq. (2.11) is then the probability that a site on the plane z belongs to a finite cluster and

$$\varphi(z) = 1 - W(z) \tag{2.12}$$

is the z-dependent percolation probability, i.e., the probability that a site on the plane z belongs to an infinite cluster.

The probability W that *any* site belongs to a finite cluster is obtained from Eq. (2.11) and the definition of $\gamma_z(\xi_z)$:

$$W = \frac{1}{L}\sum_z W_z$$

$$= \frac{1}{L}\sum_{\xi_0,\ldots,\xi_L=1}^{M}[\xi_0 + \xi_1 + \cdots + \xi_L]\gamma(\xi_0, \ldots, \xi_L)$$

$$= \sum_{\xi=1}^{ML}\xi\gamma(\xi), \tag{2.13}$$

where

$$\gamma(\xi) = \sum_{\xi_0,\ldots,\xi_L=1}^{M}\frac{1}{L}\gamma(\xi_0, \ldots, \xi_L)\delta[\xi - (\xi_0 + \cdots + \xi_L)],$$

and according to Eq. (2.10), $\gamma(\xi)$ is the average number of finite clusters with ξ sites, per site. Equation (2.13) reproduces Eq. (1.1) of Ref. 3.

III. LANDAU-GINZBURG FUNCTIONAL

The Landau-Ginzburg functional for the free energy is derived by the same method we introduced in a previous paper[6] to study the order-disorder transition in a semi-infinite medium. We start by separating the bulk and surface terms in the Hamiltonian of Eq. (2.1), then

$$\beta\mathcal{H} = \beta\mathcal{H}_B + \beta\mathcal{H}_S \tag{3.1}$$

where

$$-\beta\mathcal{H}_B = \tfrac{1}{2}K_B\sum_{\vec{R},\vec{R}'}j(\vec{R} - \vec{R}')\delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'}) + \sum_{\vec{R}}h_z\delta(\sigma_{\vec{R}} - 1), \tag{3.2}$$

$$-\beta\mathcal{H}_S = \frac{1}{2}\sum_{\vec{R}_0,\vec{R}'}j(\vec{R}_0 - \vec{R}')V(z')\delta(\sigma_{\vec{R}_0} - \sigma_{\vec{R}'}), \tag{3.3}$$

with

$$j(\vec{R} - \vec{R}') = 1 \quad \text{if } |\vec{R} - \vec{R}'| = a$$

$$= 0 \quad \text{otherwise,} \tag{3.4}$$

$$V(z) = [K_{\parallel} - K_B]\delta(z) + 2[K_{\perp} - K_B]\delta(z - a)$$
$$- 2K_B\delta(z + a). \tag{3.5}$$

I call a the lattice constant and $\vec{R}_0 = (\vec{r}, 0)$ is a position vector on the surface. The function $j(\vec{R} - \vec{R}')$ in Eq. (3.3) just insures that $\beta\mathcal{K}_B$ is translational invariant and that only nearest neighbors interact.

I will not use here the representation of the q states of $\sigma_{\vec{R}}$ as the q roots of unity,[3,7] but I rather start from the identity

$$\delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'}) = \delta(\sigma_{\vec{R}} - 1)\delta(\sigma_{\vec{R}'} - 1)$$
$$+ \sum_{\sigma \neq 1} \delta[\sigma_{\vec{R}} - \sigma]\delta[\sigma_{\vec{R}'} - \sigma], \tag{3.6}$$

$$\sum_{\sigma} \delta(\sigma_{\vec{R}} - \sigma) = 1. \tag{3.7}$$

It is convenient at this point to identify the appropriate order parameter in the theory, before going to a mean-field-like approximation. From Eqs. (2.11) and (2.12) the order parameter in the bond percolation problem can be expressed

$$\varphi(z) = \left[\frac{\partial}{\partial q} \left(\frac{1}{M} \frac{\partial}{\partial h_z} \ln Q - \frac{1}{q} \right) \right]_{q=1}$$
$$= \left[\frac{\partial}{\partial q} \left(\frac{q-1}{q} \psi(z) \right) \right]_{q=1}, \tag{3.8}$$

where we used Eq. (2.7) and

$$\psi(z) = \frac{1}{q-1} \left(\frac{q}{M} \sum_{\vec{r}} \langle \delta(\sigma_{\vec{r},z} - 1) \rangle - 1 \right). \tag{3.9}$$

$\psi(z)$ in Eq. (3.9) is the correct order parameter for the q-states Potts model: in the disordered phase all the q states are equally probable and we obtain from Eq. (3.7) that $\langle \delta(\sigma_{\vec{R}} - 1) \rangle = q^{-1}$ and $\psi(z) = 0$, while in the complete ordered phase $\langle \delta(\sigma_{\vec{R}} - 1) \rangle = 1$ and $\psi(z) = 1$. To this order parameter is associated the operator

$$\Psi(z) = \frac{1}{q-1} \left(q \sum_{\vec{r}} \delta(\sigma_{\vec{r},z} - 1) - M \right). \tag{3.10}$$

To obtain mean-field theory we replace the Hamiltonian of Eq. (3.1) by an effective Hamiltonian that neglects correlations of the order parameter on the planes, but we keep the correlations between planes.[6] In other words we approximate in Eq. (3.2):

$$j(\vec{R} - \vec{R}') \approx (n/M)j(z - z'), \tag{3.11}$$

$$j(z - z') = [n_S\delta(z - z') + \delta(z - z' - a) + \delta(z - z' + a)]/n, \tag{3.12}$$

where n is the coordinate number of the lattice and $n_S = n - 2$ the coordination number on the plane. Moreover, we consider that the $q - 1$ components of $\sigma_{\vec{R}}$ that are not coupled to the field are equivalent and we also neglect the correlations between them by approximating the identity in Eq. (3.6) by

$$\delta(\sigma_{\vec{R}} - \sigma_{\vec{R}'}) \approx \delta(\sigma_{\vec{R}} - 1)\delta(\sigma_{\vec{R}'} - 1)$$
$$+ \frac{1}{q-1} \left[\sum_{\sigma \neq 1} \delta(\sigma_{\vec{R}} - \sigma) \right]\left[\sum_{\sigma' \neq 1} \delta(\sigma_{\vec{R}'} - \sigma') \right]. \tag{3.13}$$

Introducing Eqs. (3.11) and (3.13) in Eq. (3.2) we obtain the effective Hamiltonian $-\beta\mathcal{K}_B$:

$$-\beta\mathcal{K}_B = \frac{1}{2M} \frac{(q-1)}{q} K_B n \sum_{z,z'} j(z - z')\Psi(z)\Psi(z')$$
$$+ \frac{(q-1)}{q} \sum_z h_z \Psi(z), \tag{3.14}$$

where $\Psi(z)$ is as defined in Eq. (3.10) and we dropped an uninteresting constant. We expressed

$$\sum_{\sigma \neq 1} \delta(\sigma_{\vec{R}} - \sigma) = 1 - \delta(\sigma_{\vec{R}} - 1).$$

To obtain the effective surface term from Eq. (3.3) we use also Eqs. (3.11) and (3.13), but we make the further approximation[6]

$$\Psi(0)\Psi(z) \approx \Psi(0)\langle\Psi(z)\rangle, \quad z \neq 0$$
$$\Psi(0)\Psi(0) \approx 2\Psi(0)\langle\Psi(0)\rangle. \tag{3.15}$$

We obtain for the effective surface Hamiltonian

$$-\beta\mathcal{K}_S = \frac{(q-1)}{q} K_B n g_0 \Psi(0), \tag{3.16}$$

$$g_0 = \sum_{z=0}^{L} j(z)U(z)\psi(z), \tag{3.17}$$

with $\psi(z)$ as defined in Eq. (3.9) and

$$U(z) = (K_{\parallel}/K_B - 1)\delta(z) + (K_{\perp}/K_B - 1)\delta(z - a)$$
$$- \delta(z + a). \tag{3.18}$$

To evaluate the partition function from the effective Hamiltonian we use Gaussian integration techniques. From the identity

$$\exp\left(\frac{1}{2} \frac{C}{M} \sum_{z,z'} j(z - z')\Psi(z)\Psi(z') \right) = \mathfrak{N}^{-1} \int \cdots \int_{-\infty}^{\infty} \prod_{z=0}^{L} dy(z) \exp\left(-\frac{CM}{2} \sum_{z,z'} j^{-1}(z - z')y(z)y(z') + C \sum_z y(z)\Psi(z) \right)$$

$$\tag{3.19}$$

where $C = K_B n(q-1)/q$ and $\mathfrak{K}$ is a numerical constant; we obtain for the partition function

$$Q = \mathrm{Tr}[\exp(-\beta \mathcal{K}_B - \beta \mathcal{K}_S)]$$

$$= \mathfrak{K}^{-1} \int \cdots \int \prod_z dy(z) \exp\left[-\frac{CM}{2} \sum_{z,z'} j^{-1}(z - z')y(z)y(z') \right] T[\{y\}].$$ (3.20)

The function $T[\{y\}]$ is expressed by the trace

$$T[\{y\}] = \prod_{\vec{r}, z \neq 0} \mathrm{Tr}[\sigma_{\vec{r},z}] \exp\{[\delta(\sigma_{\vec{r},z} - 1) - q^{-1}][h_z + K_B n y(z)]\} \prod_{\vec{r}} \mathrm{Tr}\{\sigma_{\vec{r},0}\} \exp\{[\delta(\sigma_{\vec{r},0} - 1) - q^{-1}][h_0 + K_B n \nu_0 y_0]\},$$

(3.21)

where

$$\nu_0 = 1 + g_0/y_0.$$ (3.22)

The trace is now easily performed and the partition function in Eq. (3.20) can be written

$$Q = \mathfrak{K}^{-1} \int \cdots \int_{-\infty}^{\infty} \prod_z dy(z) \exp[-M(G_B + G_S)],$$

(3.23)

where

$$G_B = \tfrac{1}{2} K_B n \frac{(q-1)}{q} \sum_{z,z'} j^{-1}(z - z')y(z)y(z')$$

$$+ \sum_{z=0}^{L} \left(\frac{K_B n}{q} y(z) - \ln\{\exp[h_z + K_B n y(z)] + (q-1)\} \right),$$ (3.24)

$$G_S = \frac{K_B n}{q}(\nu_0 - 1)y(0)$$

$$- \ln \frac{\exp[h_0 + K_B n \nu_0 y(0)] + (q-1)}{\exp[h_0 + K_B n y(0)] + (q-1)}.$$ (3.25)

From Eqs. (3.9) and (3.24) the order parameter $\psi(z)$ is given by

$$\psi(z) = \frac{1}{(q-1)}\left(q \frac{1}{M} \frac{\partial}{\partial h_z} \ln Q - 1 \right)$$

$$= (q-1)^{-1} \left\langle -\frac{1}{K_B n} \frac{\partial G_B}{\partial y(z)} \right.$$

$$\left. + (q-1) \sum_{z'} j^{-1}(z-z')y(z') \right\rangle,$$ (3.26)

where

$$\langle A(\{y(z)\}) \rangle$$

$$= Q^{-1} \int \cdots \int \prod dy(z)$$

$$\times \exp[-M(G_B + G_S)] A(\{y(z)\}).$$

The Landau-Ginzburg functional is obtained in the continuum limit of Eq. (3.24). We write[6]

$$y(z)y(z') \approx y^2(\bar{z}) - \left(\frac{dy}{dz}\right)^2 \frac{(z-z')^2}{4},$$ (3.27)

where $\bar{z} = (z + z')/2$ and we neglect higher derivatives. Hence Q is given by the functional integral, in zero field

$$Q = \int \delta y(z) \exp[-M(G_B + G_S)],$$ (3.28)

where, in the limit $L \to \infty$, G_B is expressed by the integral

$$G_B = \frac{1}{a} \int_0^\infty dz\, G_B(y(z)),$$ (3.29)

$$G_B(y(z)) = \frac{1}{4} \frac{(q-1)}{q} K_B a^2 \left(\frac{dy}{dz}\right)^2 + V_B(y(z)),$$ (3.30)

$$V_B(y) = \frac{1}{2} \frac{(q-1)}{q} K_B n y^2 + \frac{K_B n}{q} y - \ln[e^{K_B n y} + (q-1)],$$

(3.31)

and G_S is unchanged. In the limit $M \to \infty$, Q is evaluated by steepest descents and $y(z)$ is given by the stationary condition

$$\frac{\delta}{\delta y(z)}(G_B + G_S) = 0,$$ (3.32)

where $\delta/\delta y(z)$ is a functional derivative. We obtain from Eqs. (3.29) and (3.30)

$$\frac{(q-1)}{q} \frac{a^2}{2n} \frac{d^2 y}{dz^2} - \frac{1}{K_B n} V_B'(y(z)) = 0,$$ (3.33)

$$\frac{(q-1)}{q} \frac{a}{2n} \left(\frac{dy}{dz}\right)_{z=0} - \frac{1}{K_B n} G_S'(y(0)) = 0,$$

$$\left(\frac{dy}{dz}\right)_{z=\infty} = 0.$$ (3.34)

A steepest descent evaluation of the order parameter $\psi(z)$ in Eq. (3.26) gives, from Eq. (3.32),

$$\psi(z) = \sum_{z'} j^{-1}(z - z')y(z') \approx y(z), \qquad (3.35)$$

where $y(z)$ satisfies the stationary condition of Eq. (3.32).

Equation (3.33) is then the differential equation for the order parameter in the q-states Potts model, with the boundary condition at the surface given by Eq. (3.34). The standard mean-field theory[7] for a uniform medium is obtained by neglecting the surface term and by writing $y(z) = R$, independent of z. It follows from Eq. (3.32) that

$$R = [e^{K_B n R} - 1][e^{K_B n R} + (q - 1)]^{-1},$$

and the mean-field free energy of Mittag and Stephen[7] is reproduced by introducing this expression for R in Eq. (3.31).

For $q \geq 3$, Eqs. (3.33) and (3.34) cannot be solved by standard analytical methods[6,9] because mean-field theory predicts in this case a first-order transition[7] that cannot be described by a perturbation expansion in the order parameter close to the transition point. For $q = 2$ we recover the Landau-Ginzburg equations for the Ising model, that have been widely investigated.[9] In the limit $q = 1$, the percolation transition is again continuous and Eq. (3.33) can be integrated to obtain $y(z)$ close to the transition. We do that in the next section.

IV. LANDAU-GINZBURG EQUATIONS FOR BOND PERCOLATION

The order parameter in the bond percolation problem is, from Eq. (3.8),

$$\varphi(z) = [\psi(z)]_{q=1} = [y(z)]_{q=1}, \qquad (4.1)$$

and from Eqs. (3.33) and (3.34) it is the solution of the differential equation

$$\frac{a^2}{2n} \frac{d^2 y}{dz^2} - \frac{1}{K_B n} F_B'(y(z)) = 0 \qquad (4.2)$$

with boundary conditions

$$\frac{a}{2n}\left(\frac{dy}{dz}\right)_{z=0} - \frac{1}{K_B n} F_S'(y(0)) = 0; \quad \left(\frac{dy}{dz}\right)_{z=\infty} = 0. \qquad (4.3)$$

Here F_B and F_S are defined to be

$$F_B(y) = \lim_{q \to 1}\left[\frac{1}{q-1} V_B(y)\right]$$

$$= \tfrac{1}{2} K_B n y^2 - K_B n y - e^{-K_B n y}; \qquad (4.4)$$

$$F_S(y) = \lim_{q \to 1}\left[\frac{1}{q-1} G_S(y)\right]$$

$$= e^{-K_B n y(0)} - e^{-K_B n \nu_0 y(0)} - K n(\nu_0 - 1)y(0) \qquad (4.5)$$

and we used Eqs. (3.25) and (3.31). From Eqs. (2.7) and (3.28), we can identify $F_B(y)$ in Eq. (4.4) as the mean-field approximation for $F(h = 0)$ in a uniform infinite system, when y is independent of z. In the physical region of the order parameter, $0 \leq y \leq 1$, $F_B(y) < 0$ and it has the correct sign. When $K_B n < 1$, $F_B(y)$ has a minimum at $y = 0$ and a maximum for $y < 0$, while for $K_B n > 1$ it has a maximum at $y = 0$ and a minimum for some $0 < y_B < 1$. The transition is continuous and it can be studied by expanding $F_B(y)$ and $F_S(y)$ up to the third and second power, respectively. We obtain from Eqs. (4.2) and (4.3)

$$\frac{d^2 y}{dz^2} = \frac{(K_B n)^2}{a^2} n(ty + y^2), \qquad (4.6)$$

$$\left(\frac{dy}{dz}\right)_{z=0} = \lambda^{-1} y(0); \quad \left(\frac{dy}{dz}\right)_{z=\infty} = 0, \qquad (4.7)$$

where

$$t = 2(1 - K_B n)/(K_B n)^2 \approx 2(1 - K_B n), \qquad (4.8)$$

$$\lambda^{-1} = -(\nu_0^2 - 1)(2n/a)(K_B n). \qquad (4.9)$$

The last expression in Eq. (4.8) is justified because we are working in the region $|dy/dz| \ll 1/a$, for the continuum approximation to be valid, and this will imply that $|t| \ll 1$ or $K_B n$ close to unity. In Eq. (4.9), λ^{-1} is the "surface force" or inverse extrapolation length. Also the validity of this theory is restricted to $\lambda^{-1} \ll 1/a$ or ν_0 close to unity. Introducing Eqs. (3.17) and (3.18) in the definition of ν_0 in Eq. (3.22) we obtain

$$\nu_0^2 - 1 \approx 2(\nu_0 - 1)$$

$$= \frac{2}{K_B n}[(K_\parallel - K_B)n_S + (K_\perp - K_B) - K_B], \qquad (4.10)$$

where we approximated $\psi(z) = y(z) \approx y(0)$ and $j(z)$ is given in Eq. (3.12).

The first integral[9] of Eq. (4.6) is obtained by multiplying both sides of the equation by $\int_z^\infty (dy/dz')dz'$ and by using the boundary condition at $z = \infty$:

$$\left(\frac{dy}{dz}\right)^2 = \frac{2n}{a^2}(K_B n)^2[\tfrac{1}{2} t y^2 + \tfrac{1}{3} y^3 + \Theta(-t)|t|^3/6], \qquad (4.11)$$

where $\Theta(-t)$ is the unit step function and

$$y_B = y(z \to \infty) = \Theta(-t)|t| \qquad (4.12)$$

is the value of the order parameter in the bulk. The order parameter at the surface is one of the solutions of the cubic equation, from Eqs. (4.11) and (4.7)

$$\tfrac{1}{3} y_0^3 + t y_0^2 + \Theta(-t)|t|^3/6 = 0, \qquad (4.13)$$

where

$$\tau = \tfrac{1}{2}[t - \lambda^{-2}(a^2/n)(K_B n)^{-2}] . \qquad (4.14)$$

We do not go into the tedious details of the solution of a cubic equation and we just quote the results here. Equation (4.13) has three real solutions:

$$y_1 = -\tau(2\cos\alpha + 1) ,$$

$$y_2 = -\tau[2\cos(\alpha + \tfrac{2}{3}\pi) + 1] , \qquad (4.15)$$

$$y_3 = -\tau[2\cos(\alpha - \tfrac{2}{3}\pi) + 1] ,$$

where

$$\alpha = \Theta(-t)\tfrac{1}{3}\arctan[\Delta(|\tau|^3 - |t|^3/4)^{-1}] , \qquad (4.16)$$

$$\Delta^2 = \tfrac{1}{2}|t|^3[|\tau|^3 - \tfrac{1}{8}|t|^3] > 0 . \qquad (4.17)$$

The physical solution for the order parameter at the surface y_0 depends on the signs of t, τ, and λ^{-1}. We distinguish two main regions and we present the results obtained by integrating Eq. (4.11):

$$z = \pm\frac{a}{K_B n}\frac{1}{\sqrt{n}}\int_{y(z)}^{y_0} dy\,(ty^2 + \tfrac{2}{3}y^3 + \tfrac{1}{3}y_B^3)^{-1/2} , \qquad (4.18)$$

where y_B was defined in Eq. (4.12).

Region I. $\lambda^{-1} < 0$. From the boundary condition in Eq. (4.7), $y(0) \geqslant y(z) \geqslant y_B$ and equation (4.18) should be considered with the positive sign.
(a) $t > 0, \tau > 0$;

$$y_2 = y_3 = 0 , \quad y_0 = y_B = y(z) = 0 . \qquad (4.19)$$

(b) $t > 0, \tau < 0$;

$$y_B = 0 ; \quad y_0 = y_1 = 3|\tau| ; \qquad (4.20)$$

$$y(z) = \tfrac{3}{2}t[\sinh(z/\xi + U_0)]^{-2} , \qquad (4.21)$$

$$\xi = 2(a/\sqrt{n})|t|^{-1/2} , \qquad (4.22)$$

$$U_0 = \arg\sinh(\tfrac{1}{2}t/|\tau|)^{1/2} . \qquad (4.23)$$

(c) $t < 0, \tau < 0$.
For these values of t and τ, we check from Eq. (4.15) the inequalities $y_2 < 0 < y_3 < y_B < y_1$, when $0 \leqslant \alpha \leqslant \tfrac{1}{6}\pi$. Hence we obtain

$$y_0 = y_1 = |\tau|(2\cos\alpha + 1) ; \quad y_B = |t| \qquad (4.24)$$

$$y(z) = y_B + \tfrac{3}{2}|t|[\sinh(z/\xi + U_0')]^{-2} , \qquad (4.25)$$

where now

$$U_0' = \arg\sinh[\tfrac{2}{3}(y_0/|t| - 1)]^{-1/2} , \qquad (4.26)$$

and ξ is given by Eq. (4.22).

Region II. $\lambda^{-1} > 0$. From the boundary condition in Eq. (4.7), $y(0) \leqslant y(z) \leqslant y_B$ and we consider Eq. (4.18) with negative sign. (a) $t > 0$; $y_0 = y(z) = y_B = 0$. (b) $t < 0, \tau < 0$;

$$y_0 = y_3 = |\tau|[2\cos(\alpha - \tfrac{2}{3}\pi) + 1] < y_B , \qquad (4.27)$$

$$y(z) = y_B - \tfrac{3}{2}|t|[\cosh(z/\xi + U_0'')]^{-2} , \qquad (4.28)$$

$$U_0'' = \arg\cosh[\tfrac{2}{3}(1 - y_0/|t|)]^{-1/2} . \qquad (4.29)$$

When $\lambda^{-1} = 0$, the effect of the surface disappears and $\tau = \tfrac{1}{2}t$. In this case we obtain from Eqs. (4.15)–(4.17) that $\alpha = \Theta(-t)\pi/3$ and $y_1 = y_3 = |t| = y_B$ when $t < 0$. The regions I(c) and II(b) coincide and we have from both Eqs. (4.25) and (4.28) $y(z) = y_B = |t|$.

We summarize the results in terms of the occupation probabilities p_α, $\alpha = B$, $\|$, or $\perp$, by using Eq. (2.6). We write from Eqs. (4.8)–(4.10)

$$t = 2n\ln(q_B/q_c) ,$$

$$\lambda^{-1} = -\frac{2n}{a}[2n\ln(q_B/q_c) - 2\ln(q_\|^{ns}q_\perp/q_c^n)]$$

$$= \frac{2n}{a}(\omega - t) , \qquad (4.30)$$

where $q_\alpha = 1 - p_\alpha$, $K_\alpha = \ln(q_\alpha^{-1})$ and $q_c = e^{-1/n}$ is the mean-field value[3] for the percolation concentration of vacancies in the bulk. Here

$$\omega = 2\ln[q_\|^{ns}q_\perp/q_c^n] , \qquad (4.31)$$

and from Eq. (4.14)

$$\tau = \tfrac{1}{2}(K_B n)^{-2}[t - 4n(\omega - t)^2] . \qquad (4.32)$$

When $\lambda^{-1} < 0, t > \omega$ and the concentration of vacancies is higher in the bulk that on the surface. When $q_B > q_c$ it follows that $t > 0$ and we can define a critical value of ω from Eq. (4.32):

$$\omega_S(q_B) = -\tfrac{1}{2}(t/n)^{1/2} = -[\tfrac{1}{2}\ln(q_B/q_c)]^{1/2} < 0 \qquad (4.33)$$

such that $\operatorname{sgn}(\tau) = \operatorname{sgn}(\omega - \omega_S)$. We then obtain in region I: (i) $q_B > q_c$, $\omega > \omega_S(q_B)$ and all clusters are finite; (ii) $q_B > q_c$, $\omega < \omega_S(q_B)$. The concentration of vacancies on the surface is sufficiently small that there is a finite probability for a cluster to form in the neighborhood of the surface. The magnitude of $\omega_S(q_B)$ decreases with q_B, then the closer q_B is to q_c the less bonds are needed on the surface for a surface transition to occur. (iii) $q_B < q_c$, and there is also a finite probability for an infinite cluster to form in the bulk, but the probability for an infinite cluster remains enhanced at the surface. In region II $t < \omega$ and the excess of vacancies on the surface prevents the surface from ordering independently of the bulk: (i) $q_B > q_c$ and all clusters are finite; (ii) $q_B < q_c$ and there is a finite probability for an infinite cluster to form in the system, but this probability is larger in the bulk that on the surface.

Following Lubensky and Rubin,[9] we can identify regions I(ii), I(iii), and II(ii) as describing a "surface" transition, an "extraordinary" transition, and the "ordinary" transition. According-

ly, we define the critical exponents β_1^i and β_∞^i, where $i = s, e, o$ stands for surface, extraordinary, and ordinary.

We obtain from Eqs. (4.20) and (4.32) for the surface transition

$$y_0(t) = (t_S - t)^{\beta_1^s} ; \quad t_S \approx 4n\omega^2 , \quad \omega < 0 ;$$

$$\beta_1^s = 1; \quad \beta_\infty^s \text{ undefined} . \tag{4.34}$$

From Eqs. (4.24) and (4.16) we obtain for the extraordinary transition

$$y_0(t) - y_0(0) = |t|^{\beta_1^e} ; \quad y_B(t) = |t|^{\beta_\infty^e} ;$$

$$\beta_1^e = 1; \quad \beta_\infty^e = 1 ; \tag{4.35}$$

and from Eqs. (4.27) and (4.16), for the ordinary transition

$$y_0(t) = |t|^{\beta_1^o} ; \quad y_B(t) = |t|^{\beta_\infty^o} ,$$

$$\beta_1^o = \tfrac{3}{2}; \quad \beta_\infty^o = 1 . \tag{4.36}$$

Bray and Moore[10] have shown that surface exponents can be derived exactly in terms of bulk exponents. From Eqs. (4.4) and (4.12) $F_B(t)$ $\approx |t|^{2-\alpha}$ with $\alpha = -1$; while from Eq. (4.22) $\nu = \tfrac{1}{2}$. It follows that β_1^o in Eq. (4.36) satisfies the scaling relation $\beta_1 = \tfrac{1}{2}(3 - \alpha) - \nu$. The validity of the continuum theory is restricted to $\lambda, \xi \gg a$, where ξ is the bulk correlation length in Eq. (4.22), then to $|t| \ll 1$, $|\omega| \ll 1$.

V. CONCLUSIONS

I have analyzed the q-states Potts model in a semi-infinite medium within the context of mean-field theory by deriving the Landau-Ginzburg free-energy functional for the order parameter.

The differential equations for the order parameter are explicitly solved in the limit $q = 1$, when the Potts model represents the bond percolation model, as is shown in Sec. II. I demonstrate in Sec. II that a percolation probability $\varphi(z)$ for a given plane z can be rigorously defined by introducing z-dependent external fields in the Potts Hamiltonian. Here $\varphi(z)$ is the probability that a site on the plane z belongs to an infinite cluster. I consider in general that the occupation probabilities of bonds are different in the bulk than on the surface. The results obtained are analogous than those obtained previously for the Ising model.[6,9] We can define an inverse extrapolation length or surface force λ^{-1} that depends on the bulk and surface concentration of bonds. According to its being positive or negative a surface transition may or may not occur. In this theory a transition occurs when an infinite cluster starts to form in the system and in a surface transition the infinite cluster is concentrated in the neighborhood of the surface, while in the bulk only finite clusters occur, i.e., $\varphi(z \to \infty) = 0$.

The detailed results in terms of occupation probabilities were analyzed at the end of Sec. IV.

[1]A. G. Dunn, J. W. Essam, and J. M. Loveluck, J. Phys. C 8, 743 (1975).

[2]J. W. Essam, K. M. Gwilym, and J. M. Loveluck, J. Phys. C 9, 365 (1976).

[3]M. J. Stephen, Phys. Rev. B 15, 5674 (1977); A. B. Harris, T. C. Lubensky, W. K. Holcomb, and C. Dasgupta, Phys. Rev. Lett. 35, 327 (1975).

[4]M. R. Giri, M. J. Stephen, and S. S. Grest, Phys. Rev. 16, 4971 (1977).

[5]C. M. Fortuin and P. W. Kasteleyn, Physica 57, 536 (1972).

[6]A. Theumann and K. H. Bennemann, Phys. Rev. B 17, 331 (1978).

[7]L. Mittag and M. Stephen, J. Phys. A 9, L109 (1974).

[8]S. Alexander and D. J. Amit, J. Phys. A 8, 1988 (1975); S. Alexander, Solid State Commun. 14, 1069 (1974).

[9]T. C. Lubensky and M. H. Rubin, Phys. Rev. B 12, 3885 (1975), and references therein. See also K. Binder and P. C. Hohenberg, Phys. Rev. B 6, 3461 (1972); 9, 2194 (1974).

[10]A. J. Bray and M. A. Moore, Phys. Rev. Lett. 38, 1046 (1977).