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Surface effects and percolation : the repulsive case

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Résumé. — On calcule les exposants σ et γ_1 , respectivement reliés au profil du paramètre d'ordre et à la susceptibilité de surface, au premier ordre en $\varepsilon = 6 - d$ pour le point fixe en φ^3 du modèle de Potts — qui contient le problème de la percolation — dans un milieu semi-infini avec paroi répulsive. Les résultats sont compatibles avec les arguments de *scaling* dus à Bray et Moore.

Abstract. — The exponents σ and γ_1 , respectively related to the profile of the order parameter and to the surface susceptibility, are calculated to first order in $\varepsilon = 6 - d$ for the φ^3 fixed point of the Potts model — which contains the percolation problem — in a semi-infinite medium with a repulsive wall. The results agree with Bray and Moore's scaling arguments.

Surface effects in percolation problems turn out to be important in various physical situations, among which we shall quote a few examples : injection of a fluid into a porous medium by applying a pressure on the surface [15], adherence of a gel to a wall [18], plug flow of a fluid containing particles in suspension [9], etc... There exists an abundant literature concerning critical phenomena in semi-infinite media [1], which proposes mean-field approximations [2, 3], scaling theories [4, 5], renormalization group treatments [6, 7], etc... Besides, percolation near the threshold has been known for a long time to pertain to critical phenomena in particular through equivalences with the Potts model [8]. These equivalences can be used to study the surface behaviour of systems showing percolation. The Ginzburg-Landau theory of this problem has recently been investigated in an extensive way by A. Theumann [10]. Numerical simulations are now in progress [16]. A $6 - d$ analysis will be presented here, focusing on the most accessible features, namely the profile of the order parameter (percolation probability) and the surface susceptibility (mean cluster size near the surface).

The modification of the interaction on the surface is measured by a parameter λ , called the extrapolation length [1, 3]. The repulsive case $\lambda \geq 0$ and the attractive case $\lambda < 0$ are qualitatively different. In the latter the surface is expected to order before the bulk for sufficiently high space dimension ; then, when the

bulk orders, scaling theories [3] claim that the order parameter behaves near the surface like

$$\psi(z) \sim (z + |\lambda|)^{-\beta/\nu}$$

where β and ν are the bulk exponents. In the repulsive case a new exponent σ appears [12] :

$$\psi(z) \sim \psi(\infty) \left(\frac{z + \lambda}{\xi} \right)^\sigma. \quad (1)$$

This letter will only deal with the repulsive case.

With a view to a renormalization treatment the bond percolation model is converted into the continuum version of the Potts model, namely a field theory described by the following Lagrangian or Ginzburg-Landau functional [11] :

$$\begin{aligned} \mathcal{L} = \int_{\mathcal{D}} d^d x \left[\frac{1}{2} r_0 \varphi_x^2(x) + \frac{1}{2} |\nabla \varphi_x(x)|^2 + \right. \\ \left. + \frac{1}{3!} g_0 D_{\alpha\beta\gamma} \varphi_\alpha(x) \varphi_\beta(x) \varphi_\gamma(x) + \frac{1}{2} \lambda^{-1} \delta(z) \varphi_x^2(x) \right]. \quad (2) \end{aligned}$$

The integral over the position variable $x = (\rho, z)$ is extended to the semi-infinite domain $\mathcal{D}$ defined by $z \geq 0$, ρ being the projection of x on the surface

$z = 0$; φ is a n -dimensional vector field, n being related to the underlying s -states Potts model by $s = n + 1$. The percolation problem is obtained in the limit $n \rightarrow 0$, as far as cluster properties are concerned. The interaction tensor is

$$D_{\alpha\beta\gamma} = \sum_{\lambda} e_{\alpha}^{\lambda} e_{\beta}^{\lambda} e_{\gamma}^{\lambda}$$

where the vectors e^{λ} ($\lambda = 1, \dots, n + 1$) generate a hypertetrahedron :

$$e^{\lambda} \cdot e^{\mu} = (n + 1) \delta_{\lambda\mu} - 1.$$

Terms in φ of order higher than three, which have been proved to be irrelevant to the percolation ($n = 0$) case, have been omitted in (1). Lubensky and Rubin [6] have shown that, in the n -vector model, λ is unaffected by renormalization (at least to order ε). It is probably not true in the case of a cubic invariant like in (2) : the calculation below fails to yield a scaling solution $\psi(z)$ for general $\lambda > 0$ [17]. Thus one is led to work with a fixed point value λ^* , appropriate to the repulsive case, which turns out to be $\lambda^* = 0$ as will be shown in the following (the existence of an other λ^* is unlikely on physical grounds).

1. Order parameter (exponents σ and β_1). — We first set $\lambda = 0$. According to scaling predictions one looks for a profile of the order parameter ψ of the form [12]

$$\psi(x) \sim (z/\xi)^{\sigma} \psi(\infty), \quad z \ll \xi \quad (3)$$

where ξ and $\psi(\infty)$ are respectively the correlation length and the order parameter value in the bulk. Recall that when $n \rightarrow 0$, $\psi(x)$ gives the probability that site x belongs to an infinite cluster. When $d \geq 6$, mean-field theory holds and we know that $\sigma = 1$. Below six dimensions an $\varepsilon = 6 - d$ expansion of σ can be sought.

At the critical point the free energy as a functional of ψ is

$$F = \int_{\mathcal{D}} d^d x \int_{\mathcal{D}} d^d x' \Gamma_{\alpha\beta}^{(2)}(x, x') \psi_{\alpha}(x) \psi_{\beta}(x') + \text{higher order terms}.$$

$\Gamma^{(2)}$ (vertex function) is the inverse (in the matrix sense) of the correlation function. Near to the surface $z = 0$, the order parameter is small and the equation for ψ , namely $\frac{\partial F}{\partial \psi(x)} = 0$, is linearized to give

$$(r_0^* - \nabla^2) \psi_{\alpha}(x) - \int_{\mathcal{D}} d^d x' \Sigma_{\alpha\beta}^*(x, x') \psi_{\beta}(x') = 0 \quad (4)$$

where Σ is the self-energy; the stars indicate that the

quantities are taken at their fixed point values. To second order in g_0 , Σ is given by (diagram of fig. 1)

$$\begin{aligned} \Sigma_{\alpha\beta}(x, x') &= \frac{1}{2} (n + 1)^2 (n - 1) g_0^2 [G_0(x, x')]^2 \delta_{\alpha\beta} \\ &= \sigma_n g_0^2 [G_0(x, x')]^2 \delta_{\alpha\beta} \end{aligned}$$

G_0 being the free propagator in the semi-infinite medium which is expressed in terms of G_0^B , the free propagator in the translationally invariant medium (bulk), by [3]

$$G_0(x, x') = G_0^B(x, x') - G_0^B(x, vx')$$

where vx' is the *image* of x'

$$vx' = v(\rho', z') = (\rho', -z').$$

r_0^* is the same as in the bulk system :

$$r_0^* = \sigma_n g^{*2} \int \frac{d^d q}{(2\pi)^d} G_0^B(q) G_0^B(-q).$$

Fig. 1. — Self-energy graph to second order in g_0 .

When $d = 6$, the solution of (4) is $\psi_0(x) = z$. For d close to 6 the solution of (4) is calculated to first order in ε by perturbation with respect to g^* :

$$\psi(x) = \psi_0(z) + g^{*2} \psi_1(z).$$

ψ_1 is given by

$$-\frac{d^2 \psi_1}{dz^2} = \sigma_n \int_{\mathcal{D}} d^6 x' [G_0(x, x')]^2 \psi_0(z') - \frac{r_0^*}{g^{*2}} \psi_0(z). \quad (5)$$

The right hand side of (5) is calculated in Appendix I; one finds :

$$\frac{d^2 \psi_1}{dz^2} = \frac{1}{8} \sigma_n K_5 \frac{1}{z}$$

which, taking into account the condition $\psi(\xi) = 1$, is integrated to give :

$$\begin{aligned} \psi(z) &\sim (z/\xi) \left(1 + \frac{1}{8} \sigma_n K_5 g^{*2} \ln z/\xi \right) \\ &\sim (z/\xi)^{\sigma}. \end{aligned}$$

This leads to the identification of the expansion of σ

$$\sigma = 1 + \frac{1}{8} \sigma_n K_5 g^{*2} + \dots$$

Recalling that [11, 13]

$$g^{*2} = 2 \varepsilon [K_6(n+1)^2 (7-3n)]^{-1}$$

and $K_5/K_6 = 16/3$:

$$\sigma = 1 + \frac{2}{3} \frac{n-1}{7-3n} \varepsilon + \dots$$

The scaling relation (3) implies that $\beta_1 = \beta + \sigma\nu$ where β_1 is the surface exponent for the order parameter, β and ν the usual bulk exponents; hence the ε expansion of β_1 :

$$\beta_1 = 3/2 + \frac{n+11}{3n-7} \frac{\varepsilon}{12} + \dots$$

For $\lambda \neq 0$ one can prove that

$$\frac{d^2\psi_1}{dz^2} = \frac{1}{8} \sigma_n K_5 \frac{1}{z+\lambda} \left(1 + 0\left(\frac{\lambda^2}{z^2}\right) \right)$$

(the corresponding calculations will appear in a more detailed paper). With the boundary condition

$$\frac{d\psi}{dz}(0) = \lambda^{-1} \psi(0),$$

one obtains [19] :

$$\psi(z) \sim \left(\frac{z + \sigma\lambda}{\xi} \right)^\sigma \quad a \ll z \ll \xi \quad (6) \quad \lambda \ll z$$

2. Surface susceptibility (exponent γ_1). — In the following we set $\lambda = 0$. In the theory of critical phenomena in semi-infinite medium the local response $\chi(x)$ to a uniform field is considered :

$$\chi(x) = \int_{\mathcal{D}} d^d x' G(x, x')$$

$\chi(x)$ is expected to diverge at the critical point :

$$\chi(\rho, z) \sim t^{-\gamma_1} \quad z \ll \xi.$$

In percolation theory $\chi(x)$ represents the mean size of the cluster to which site x belongs.

We write $\mathcal{L}$ as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ and take for the free part $\mathcal{L}_0$

$$\mathcal{L}_0 = \int_{\mathcal{D}} d^d x \left[\frac{1}{2} r \varphi_x^2(x) + \frac{1}{2} |\nabla \varphi_x|^2 \right],$$

introducing the *renormalized mass* r , i.e. the inverse susceptibility in the bulk system : $r \sim t^\nu$.

From Dyson's equation for G

$$G(x, x''') = G_0(x, x''') +$$

$$+ \int_{\mathcal{D}} d^d x' d^d x'' G_0(x, x'') \bar{\Sigma}(x'', x') G(x', x'''),$$

we derive the equation for χ :

$$\chi(x) = \chi_0(x) + \int_{\mathcal{D}} d^d x' d^d x'' G_0(x, x'') \bar{\Sigma}(x'', x') \chi(x').$$

G_0 is conveniently given by its Fourier transform parallel to the surface :

$$\hat{G}_0(k, z, z') = \frac{1}{2p(k)} [\exp - p(k) |z' - z| - \exp - p(k) (z' + z)] \quad (7)$$

setting $p(k) = (r + k^2)^{1/2}$.

Define

$$\chi_0(z) = \int_{\mathcal{D}} d^d x' G_0(x, x') = r^{-1} (1 - \exp - r^{1/2} z); \quad (8)$$

to first order in ε we have $\chi(z) = \chi_0(z) + g^{*2} \chi_1(z)$ and

$$g^{*2} \chi_1(z) = \int_0^\infty dz'' \hat{G}_0(0, z, z'') \int d^{d-1} \rho' \times \int_0^\infty dz' \bar{\Sigma}(\rho' - \rho'', z'', z') \chi_0(z') \quad (9)$$

χ_1 is calculated in the small r limit in Appendix II :

$$\chi_1(z) \sim -\frac{5}{32} \sigma_n K_5 r^{-1/2} z \ln r^{-1/2}$$

and thus

$$\chi(z) \sim r^{-1/2} z \left(1 - \frac{5}{32} \sigma_n K_5 g^{*2} \ln r^{-1/2} + \dots \right).$$

Finally, knowing that $\gamma \simeq 1 + \frac{n-1}{3n-7} \varepsilon + \dots$, we find :

$$\gamma_1 = \frac{1}{2} \left(1 + \frac{11}{6} \frac{n-1}{3n-7} \varepsilon + \dots \right).$$

3. Conclusion. — Setting $n = 0$ in the previous results we obtain the percolation exponents :

$$\sigma = 1 - \frac{2\varepsilon}{21} + \dots, \quad \beta_1 = 3/2 - \frac{11\varepsilon}{84} + \dots,$$

$$\gamma_1 = 1/2 + \frac{11\varepsilon}{84} + \dots$$

The formulas for β_1 and γ_1 agree for all n with the expansions obtained from scaling relations : these relations, including Bray and Moore's prediction $\gamma_{1,1} = \nu - 1$, allow to calculate all the surface exponents from the bulk exponents [7] :

$$\beta_1 = \frac{1}{2} + \frac{1}{2} \nu(d-2) \quad \gamma_1 = \nu + \frac{1}{2} (\gamma - 1).$$

The *ordinary* transition [2, 7] has only been considered here. Other questions are still to be studied, in particular the attractive case and the possibility for a surface transition which has recently been suggested [10, 14].

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Appendix I. — We calculate the quantity

$$\phi(z) = \int_0^\infty dz' \int d^5\rho' [G_0(\rho, z; \rho', z')]^2 z'.$$

Let us introduce the Fourier transform of G_0 with respect to $\rho - \rho'$ [7, 3]

$$\begin{aligned} \hat{G}_0(k, z, z') &= \int d^5(\rho - \rho') G_0(\rho, z; \rho', z') e^{ik(\rho - \rho')} \\ &= \frac{1}{2|k|} [\exp - |k||z - z'| - \exp - |k|(z + z')]. \end{aligned}$$

Then

$$\phi(z) = \int \frac{d^5k}{(2\pi)^5} \int_0^\infty dz' \hat{G}_0(k, z, z') \hat{G}_0(-k, z, z') z'.$$

After performing the integration over z' one gets :

$$\phi(z) = \int \frac{d^5k}{(2\pi)^5} \frac{1}{4|k|^2} [z/|k| - z^2 e^{-2|k|z} - z/|k| e^{-2|k|z}].$$

On the other hand

$$\frac{r_0^*}{g^{*2} \sigma_n} = \int \frac{d^5k}{(2\pi)^5} \int_{-\infty}^{+\infty} dz \hat{G}_0^B(k, z) \hat{G}_0^B(-k, z) = \int \frac{d^5k}{(2\pi)^5} \frac{1}{4|k|^3}.$$

Equation (4) becomes :

$$\begin{aligned} -\frac{d^2\psi_1}{dz^2} &= -\frac{\sigma_n}{(2\pi)^5} \int \frac{d^5k}{4|k|^2} (z^2 e^{-2|k|z} + z e^{-2|k|z}/|k|) \\ \frac{d^2\psi_1}{dz^2} &= \frac{1}{4} \sigma_n K_5 \int_0^\infty dk k^2 (z^2 + z/k) e^{-2kz} = \frac{1}{8} \sigma_n K_5 \frac{1}{z} \end{aligned}$$

using the standard notation $K_d = [2^{d-1} \pi^{d/2} \Gamma(d/2)]^{-1}$.

The cut-off momentum has been taken infinite, which implies that the above formula is valid for z much larger than the lattice spacing.

Appendix II. — We first calculate the quantity

$$K(z'') = (g^*)^{-2} \int d^{d-1}\rho' \int_0^\infty dz' \bar{\Sigma}(\rho' - \rho'', z'', z') \chi_0(z').$$

In this case

$$\bar{\Sigma}(x'', x') = \sigma_n g^{*2} [G_0(x'', x')]^2 + (r - r_0) \delta(x'' - x').$$

Using (5) and (6) $K(z'')$ is found after integrating over z'' :

$$K(z) = \sigma_n \int \frac{d^5 k}{(2\pi)^5} \frac{r^{-1}}{4p^2} \left[\frac{1}{p} - \exp(-r^{1/2} z) \left(\frac{1}{2p - r^{1/2}} + \frac{1}{2p + r^{1/2}} \right) - \frac{1}{p} (1 - \exp(-r^{1/2} z)) + \right. \\ \left. + \exp(-2pz) \left(\frac{1}{2p - r^{1/2}} - \frac{1}{2p + r^{1/2}} - \frac{1}{p} + 2r^{-1/2} - 2z \right) \right. \\ \left. + \exp(-(2p + r^{1/2})z) \left(-2r^{-1/2} + \frac{2}{2p + r^{1/2}} \right) \right] \quad (\text{A 2.1})$$

where the explicit dependence $p(k)$ has been dropped for simplicity.

The first three terms

$$\sigma_n \int \frac{d^5 k}{(2\pi)^5} \frac{r^{-1}}{4p^2} \left(-\frac{r \exp(-r^{1/2} z)}{p(4p^2 - r)} \right) \sim -\frac{1}{16} \sigma_n K_5 \exp(-r^{1/2} z) \ln(\Lambda r^{-1/2})$$

show an ultra-violet divergence with the cut-off Λ .

Since we are interested in the small $r^{1/2} z$ limit we can write eq. (7)

$$\chi_1(z) = \frac{1}{2} r^{-1/2} \int_0^\infty dz'' [\exp(-r^{1/2} |z'' - z|) - \exp(-r^{1/2}(z'' + z))] K(z'')$$

as

$$\chi_1(z) \sim \frac{1}{2} r^{-1/2} 2 \operatorname{sh}(r^{1/2} z) \int_{r^{1/2} z}^\infty du e^{-u} K(r^{-1/2} u).$$

Expanding $e^{-r^{1/2} z} = e^{-u}$ in (A 2.1) one finds :

$$K(r^{-1/2} u) \sim -\frac{1}{8} \sigma_n K_5 \left(\frac{1}{2} \ln \Lambda r^{-1/2} + \frac{1}{u} \right),$$

so that

$$\chi_1(z) \sim -\frac{1}{8} \sigma_n K_5 r^{-1/2} z \left[\frac{1}{4} \ln(\Lambda r^{-1/2}) - \ln(z r^{1/2}) \right] \\ \sim -\frac{5}{32} \sigma_n K_5 r^{-1/2} z \ln r^{-1/2} \quad \text{for } r^{-1/2} \gg z \gg \Lambda^{-1}.$$

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- [19] Formula (6), which takes into account the actual boundary condition $\frac{d\psi}{dz}(0) = \lambda^{-1} \psi(0)$, is slightly different from the usual scaling form (1) which can be obtained with the rather phenomenological boundary condition $\psi(-\lambda) = 0$. Only in mean-field theory, are these two conditions compatible. One can reconcile the two points of view by defining a renormalized extrapolation length $\lambda_R = \sigma \lambda_0$ to first order in ε , so that $\psi(z) \sim \left(\frac{z + \lambda_R}{\xi} \right)^\sigma$.