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LETTER TO THE EDITOR

Equation of state for bond percolation in a film

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Abstract. Solutions of the mean-field theory equation of state for the order parameter of bond percolation in a film of finite thickness are presented.

The percolation problem first formulated by Broadbent and Hammersley (1957) exhibits a continuous phase transition analogous to that found in interacting spin systems (see e.g. the review by Essam 1980). Percolation in a semi-infinite system has been discussed by De'Bell and Essam (1981) who used a probabilistic approach within mean-field (MF) theory. Theumann (1979) and Carton (1980) obtained results for the semi-infinite system by exploiting the equivalence of the bond percolation problem and the q-state Potts model in the limit $q \to 1$ first noted by Kasteleyn and Fortuin (1969). In the work of Theumann (1979), the Gaussian integration method was applied to derive the Ginzburg–Landau–Wilson (GLW) differential equation with an extrapolation length boundary condition for the MF order parameter. Carton (1980) has calculated some critical exponents to first order in $\varepsilon = 6 - d$, where d is the spatial dimensionality of the system. Here we derive the differential equation for the MF order parameter of the q-state Potts model in the limit $q \to 1$, using the method which Mills (1971) applied for a simple cubic Heisenberg ferromagnet with a (100) surface. It is shown that when the limit $q = 1$ is taken, Theumann's results are obtained. The MF order parameter for a film of finite thickness is calculated.

The Hamiltonian for the q-state Potts model is

$$\mathscr{H} = -\left(\frac{q-1}{q}\right) \sum_{l} \left(h_0(l) \boldsymbol{e}_\alpha + \sum_{\boldsymbol{\delta}} K(\boldsymbol{l}, \boldsymbol{l}+\boldsymbol{\delta}) \boldsymbol{s}_{l+\delta}\right) \cdot \boldsymbol{s}_l \tag{1}$$

where the spin variables take on the values of the position vectors of the $(q-1)$-dimensional hypertetrahedron, $\boldsymbol{e}_1, \ldots, \boldsymbol{e}_q$, with $\boldsymbol{e}_\alpha \cdot \boldsymbol{e}_\beta = (q\delta_{\alpha\beta} - 1)/(q-1)$. A lattice site is denoted by $\boldsymbol{R}_l = (\boldsymbol{l}_\| a_0, l_z a_0)$ where the film is unbounded in the $\boldsymbol{l}_\|$ plane (parallel to the surfaces) and $l_z = 1, 2, 3, \ldots$ is a label for the planes parallel to the (100) surface of a simple cubic lattice with lattice spacing a_0. $h_0(l)$ is an external, static field parallel to one of the vectors $\boldsymbol{e}_\alpha$ and the interaction K is assumed to be $K_\|$ for nearest-neighbour ($\boldsymbol{l}$ and $\boldsymbol{l}+\boldsymbol{\delta}$) spins in the surface layers and K_{B} otherwise.

Within MF theory, we assume that the *net* ordering in a plane is parallel to $\boldsymbol{e}_\alpha$ by replacing $\boldsymbol{s}_{l+\delta}$ in (1) by its average value. Defining the order parameter ϕ by $\langle \boldsymbol{s}_{l+\delta} \rangle = \boldsymbol{e}_\alpha \phi(\boldsymbol{l}+\boldsymbol{\delta})$, we obtain the MF Hamiltonian

$$\mathscr{H}_{\mathrm{MF}} = -\left(\frac{q-1}{q}\right) \sum_{l} h(l) \boldsymbol{e}_\alpha \cdot \boldsymbol{s}_l \qquad h(l) \equiv h_0(l) + \sum_{\boldsymbol{\delta}} K(\boldsymbol{l}, \boldsymbol{l}+\boldsymbol{\delta}) \phi(\boldsymbol{l}+\boldsymbol{\delta}). \tag{2a, b}$$

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One may compute the order parameter by means of the equation

$$\phi(\boldsymbol{l}) = \frac{\operatorname{Tr} \boldsymbol{e}_\alpha \cdot \boldsymbol{s}_l \exp(-\mathscr{H}_{\mathrm{MF}})}{\operatorname{Tr} \exp(-\mathscr{H}_{\mathrm{MF}})} = \frac{\exp[(q-1)h/q] - \exp(-h/q)}{\exp[(q-1)h/q] + (q-1)\exp(-h/q)}, \qquad (3)$$

where the right-hand side of (3) is the analogue of the Brillouin function for a Heisenberg ferromagnet. Replacing the lattice vector $\boldsymbol{l}$ by a continuous variable $\boldsymbol{r} = (\boldsymbol{r}_\parallel, z)$ and expanding the order parameter $\phi(\boldsymbol{l}+\boldsymbol{\delta})$, calculation shows that close to the transition temperature for the film, and for l_z not a surface layer, ϕ satisfies

$$r_0(q)\phi(\boldsymbol{r}) = \nabla^2\phi(\boldsymbol{r}) + (K_{\mathrm{B}}n^2/2a_0^2q)(q-2)\phi^2(\boldsymbol{r}) + h_0(l)/a_0^2K_{\mathrm{B}} \qquad (4)$$

where

$$r_0(q) \equiv (q/a_0^2K_{\mathrm{B}})(1 - K_{\mathrm{B}}n/q) \qquad (5)$$

and n is the coordination number of the lattice. Calculation also shows that the order parameter for the surface layers satisfies (5) provided the boundary conditions

$$\left.\frac{\mathrm{d}\phi(z)}{\mathrm{d}z}\right|_{z=0(L)} = \frac{+(-)}{\Lambda}\,\phi(z)|_{z=0(L)} \qquad (6)$$

are imposed at the surfaces $z=0$ and $z=L$. The extrapolation length Λ is defined by

$$\Lambda^{-1} \equiv [(n-1)K_{\mathrm{B}} - (n-2)K_\parallel]/a_0K_{\mathrm{B}}. \qquad (7)$$

Equation (4) is not appropriate for $q>2$ since the phase transition is first order for this case (Mittag and Stephen 1974). For $q=2$ (Ising model), the coefficient of ϕ^2 in (4) vanishes and higher-order terms must be included in a discussion of the equation of state. Assuming that no external field is applied to the system so that $\phi(\boldsymbol{r})$ depends only on the variable z and setting $q=1$ in (4), we obtain the GLW equation for bond percolation in a film as

$$\mathrm{d}^2\phi(z)/\mathrm{d}z^2 = r_0\phi(z) + (K_{\mathrm{B}}n^2/2a_0^2)\phi^2(z), \qquad (8)$$

together with the boundary conditions at $z=0$ and $z=L$ which are given by (6). For convenience, we define $r_0 \equiv r_0(q=1)$. We note that in Theumann's work, the interaction ($K_\perp$) between a spin on the surface and another in the bulk could be assumed different from the interaction (K_{B}) between two spins in the bulk. In the present formalism, extrapolation length boundary conditions could only be obtained if $K_\perp$ and K_{B} are equal. Near the MF bulk transition temperature, $r_0 \ll 1$, i.e. $K_{\mathrm{B}}n \approx 1$. Making this approximation, we obtain the analogue of Theumann's equations for the order parameter. However, for a film of finite thickness, the transition temperature is shifted from its bulk value. It would not be appropriate to make the approximation $K_{\mathrm{B}}n \approx 1$ for a film.

Let $b \equiv K_{\mathrm{B}}n^2/3a_0^2$ and $u(x) = \phi_0/\phi(z)$ where variables are changed from z to x with $x = (z - L/2)(A/\phi_0^2)^{1/2}$. ϕ_0 and A are related by $r_0\phi_0^2 + b\phi_0^3 + A = 0$ where ϕ_0 is determined by the boundary conditions in (7). It is a simple matter to show that (8) may be integrated once to give

$$(\mathrm{d}u/\mathrm{d}x)^2 = u(u-1)[(u+\tfrac{1}{2})^2 - \Delta/4] \qquad (9)$$

where the discriminant $\Delta \equiv -3(1-c)/(3c+1)$ is defined in terms of c which is given by $3c = r_0/b\phi_0$. Whereas $\phi(z)$ is given in terms of the parameters A, r_0 and b, $u(x)$ is given in terms of A, ϕ_0 and c.

Case (1). For $\Delta<0$, we set $\Delta=-4\kappa^2$ where κ is real. We integrate (9) by making use of results in 3.145 of Gradshteyn and Ryzhik (1965). We obtain

$$x=(PQ)^{-1/2}F(2\tan^{-1}[Q(u-1)/Pu]^{1/2}, \tfrac{1}{2}\{[(P+Q)^2+1]/PQ\}^{1/2}), \qquad u>1, \tag{10a}$$

$$x=-(PQ)^{-1/2}F(2\tan^{-1}[-Qu/P(1-u)]^{1/2}, \tfrac{1}{2}\{[(P+Q)^2+1]/PQ\}^{1/2}), \qquad u<0, \tag{10b}$$

where $P^2=\kappa^2+\frac{9}{4}$, $Q^2=\kappa^2+\frac{1}{4}$ and F is an elliptic integral of the first kind.
Case (2). For $\Delta>0$, we set $u_\pm\equiv-\frac{1}{2}\pm\frac{1}{2}\Delta^{1/2}$. There are three temperature ranges to be considered which are determined by the order of the roots $u=0$, 1, u_+ and u_-. These temperature regions are

$$r_0<-3A\phi_0^2 \qquad \text{or} \qquad u_-<0<1<u_+, \tag{11a}$$

$$-3A\phi_0^2<r_0<-\tfrac{7}{4}A\phi_0^2 \qquad \text{or} \qquad u_-<0<u_+<1, \tag{11b}$$

$$-\tfrac{7}{4}A\phi_0^2<r_0<-\tfrac{3}{4}A\phi_0^2 \qquad \text{or} \qquad u_-<u_+<0<1. \tag{11c}$$

For each temperature range, we can integrate with the use of the results of Gradshteyn and Ryzhik (1965). For example, if $u_-<0\leqslant u<1<u_+$ we obtain

$$x=\{2/[u_+(1-u_-)]^{1/2}\}F(\sin^{-1}[u_+(1-u)/(u_+-u)]^{1/2}, [(u_+-u_-)/u_+(1-u)]^{1/2}). \tag{12}$$

Equations (10) and (12) could be written alternatively with the order parameter for a film expressed as an explicit function of the spatial coordinate where the functions involved are Jacobi elliptic functions. For example, if $\Delta>0$, $c<-\frac{1}{3}$ and $\phi_0>0$, it is straightforward to show that with $u(x)=[\psi(v)-c]^{-1}$ where $v=\frac{1}{2}x(-1-3c)^{1/2}$ we have as a solution

$$\psi(v)=a_3+(a_1-a_3)/\mathrm{sn}^2(v\sqrt{a_1-a_3}, k) \tag{13}$$

where sn is the sine amplitude Jacobi elliptic function, $k=[(a_2-a_3)/(a_1-a_3)]^{1/2}$ and $a_1>a_2>a_3$ are the roots of the cubic equation $a^3-3c^3a-(1+3c-2c^3)=0$. The solution (13) is symmetric about the mid-plane $z=L/2$ of the film. We note that for the semi-infinite system, the constant of integration A is determined by the value of the order parameter in the bulk ($z=\infty$). The value of A for the semi-infinite system gives rise to integrals which could be expressed in terms of elementary functions (Theumann 1979). For a film of finite thickness, the order parameter has been obtained in terms of the discriminant Δ which is a function of *all* the parameters for this problem.

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