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1982 J. Phys. A: Math. Gen. 15 L305

(http://iopscience.iop.org/0305-4470/15/6/010)

J. Phys. A: Math. Gen. 15 (1982) L305–L310. Printed in Great Britain

LETTER TO THE EDITOR

Non-universal and anomalous surface critical behaviour in an inhomogeneous semi-infinite Gaussian model

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Received 22 February 1982

Abstract. We consider a semi-infinite Gaussian model with spatially inhomogeneous short-range couplings which depend on the distance z from the surface. Far from the surface the coupling constants vary as $K(z)=K_B-Az^{-y}$. For $y>2$ the pair correlation function of the surface spins decays as a power law with a universal exponent $\eta_\parallel=2$ at the bulk critical temperature. For $y=2$, $\eta_\parallel$ is non-universal, and for $y<2$ there is an anomalous exponential decay.

Recently Hilhorst and van Leeuwen (1981, 1982) reported exact results for the pair correlation function $g(r)$ of the boundary spins in a semi-infinite two-dimensional Ising model with spatially inhomogeneous nearest-neighbour couplings which depend on the distance z from the surface. The coupling constants are weaker near the surface than in the bulk and vary as $K(z)=K_B-A/z^y$ for z much greater than the lattice constant. At the bulk critical temperature, for $y>1$, $g(r)$ decays as a power law with the same universal exponent $\eta_\parallel=1$ as in the homogeneous semi-infinite case $A=0$. For $y=1$, $\eta_\parallel$ is non-universal and varies continuously with A, and for $y<1$ there is an anomalous exponential decay.

It was subsequently pointed out (Burkhardt 1982a, b, Cordery 1982) that these results are compatible with a simple local scaling picture, which is applicable, in principle, to any semi-infinite system with a divergent correlation length. For a system with bulk exponent ν the scaling theory predicts†

$$g(r)\sim\begin{cases} r^{-(d-2+\eta_\parallel)} & y>\nu^{-1} \\ \exp[-(r/\tilde{\xi})^{1-\nu y}] & y<\nu^{-1}. \end{cases} \tag{1}$$

The exponent $\eta_\parallel$ for $y>\nu^{-1}$ in (1) is universal and has the same value as in the homogeneous semi-infinite case. The quantity $\tilde{\xi}$ in the anomalous exponential decay for $y<\nu^{-1}$ is a finite characteristic length at the bulk critical temperature, which according to the scaling theory varies as $\tilde{\xi}\sim A^{-\nu/(1-\nu y)}$.

† Scaling theory alone does not predict the form of the decay for $y<\nu^{-1}$, only that it involves the finite characteristic length $\tilde{\xi}$ defined below (1). An additional assumption which implies the anomalous exponential form has been discussed by Burkhardt (1982a). Another argument is as follows. In the spatially inhomogeneous system the local correlation length $\xi\sim t^{-\nu}$ varies as $\xi(z)\sim A^{-\nu}z^{\nu y}$ at the bulk critical temperature. An anomalous exponential decay of the type considered above, but perpendicular rather than parallel to the surface, arises from the combined z dependence in the ordinary exponential decay $\exp(-z/\xi(z))$, since $z/\xi(z)\sim A^{\nu}z^{1-\nu y}$.

0305-4470/82/060305+06$02.00

In this letter we consider a semi-infinite Gaussian model with inhomogeneous couplings of the type considered above. Despite the simplicity of the model, one finds the same rich variety of surface critical behaviour as y is varied as in the Ising case. Both the Gaussian and Ising results are in complete agreement with the scaling theory. In both systems in the marginal case $y=\nu^{-1}$ the exponent $\eta_\parallel$ is non-universal and varies continuously with A.

We first describe a calculation for the two-dimensional Gaussian model on a triangular lattice based on the differential real-space renormalisation method applied by Hilhorst and van Leeuwen to the Ising system. The method is only applicable to models with a star–triangle transformation. We then briefly consider an alternative approach based on a d-dimensional continuum Gaussian model.

We begin with a Gaussian model on a semi-infinite triangular lattice with partition function

$$Z=\left(\prod_\alpha\int_{-\infty}^{\infty}\mathrm{d}s_\alpha\exp(-s_\alpha^2/2)\right)\prod_{\langle\mu\nu\rangle}\exp(K_{\mu\nu}s_\mu s_\nu). \tag{2}$$

Following Hilhorst and van Leeuwen we consider nearest-neighbour couplings $K_{\mu\nu}$ of the form (see figure 1)

$$\begin{aligned} K_1(m)&=K_{1\mathrm{B}}-A_1/m^y \qquad && m=\tfrac{1}{2},\tfrac{3}{2},\ldots \\ K_2(m)&=K_{2\mathrm{B}}-A_2/m^y \qquad && m=1,2,\ldots \end{aligned} \tag{3}$$

where m gives the distance of the bond from the edge. At criticality the bulk couplings $K_{1\mathrm{B}}$, $K_{2\mathrm{B}}$ satisfy $K_{1\mathrm{B}}+2K_{2\mathrm{B}}=\frac{1}{2}$. We map the Gaussian model with coupling constants K_1, K_2 corresponding to the triangular lattice of full lines in figure 1 onto another Gaussian model with coupling constants K_1', K_2' corresponding to the triangular lattice of broken lines via an intermediate Gaussian model with couplings p_1, p_2 on the hexagonal lattice of dotted lines. The triangular lattices with couplings K_i and K_i' are generated from the hexagonal lattice by applying the star–triangle transformation (Syozi 1972, Yamazaki and Hilhorst 1979) to the right- and left-pointing stars, respectively. For the Gaussian system considered here the transformation equations have the explicit form

$$\begin{aligned} K_1(m)&=p_2(m)^2/D_+(m-\tfrac{1}{2})^2 \qquad & K_2(m)&=p_1(m)p_2(m-\tfrac{1}{2})/D_+(m-1)D_+(m) \\ K_1'(m)&=p_2(m)^2/D_-(m+\tfrac{1}{2})^2 \qquad & K_2'(m)&=p_1(m)p_2(m+\tfrac{1}{2})/D_-(m)D_-(m+1) \end{aligned} \tag{4}$$

where

$$D_\pm(m)=[1-p_1(m)^2-2p_2(m\pm\tfrac{1}{2})^2]^{1/2}. \tag{5}$$

The couplings K_i and K_i' are numbered analogously, i.e. the left-most broken vertical bond in figure 1 is $K_1'(\frac{1}{2})$.

Equations expressing the K_i' in terms of the K_i may be obtained by eliminating the p_i in (4). Iterating the transformation many times generates a sequence of triangular lattices with couplings $K_i(m,n)$, $n=0,1,2,\ldots$. The pair correlation function $g(r,n)$ of surface spins separated by r in system n transforms according to

$$g(r,n)=\tfrac{1}{4}Q(n)[g(r+1,n+1)+2g(r,n+1)+g(r-1,n+1)] \tag{6}$$

$$Q(n)=4p_2(\tfrac{1}{2},n)^2\frac{1-2p_2(\frac{1}{2},n)^2}{1-p_1(1,n)^2-2p_2(\frac{1}{2},n)^2}. \tag{7}$$

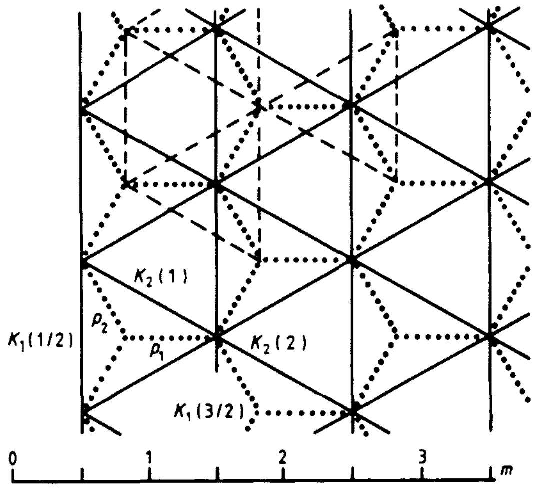

Figure 1. (After Hilhorst and van Leeuwen 1981.) The initial triangular lattice with couplings $K_1(m)$, $K_2(m)$ (full lines), the intermediate hexagonal lattice with couplings $p_1(m)$, $p_2(m)$ (dotted lines), and the new triangular lattice with couplings $K_1'(m')$, $K_2'(m')$ (broken lines, only a few triangles are shown). m is a measure of the distance from the edge. The coupling constants $K_1'(m')$, $K_2'(m')$ are numbered analogously, with $m'=\frac{1}{2}$ for the K_1' coupling furthest to the left.

Hilhorst and van Leeuwen show how to calculate the correlation function $g(r)=g(r,0)$ from the sequence of $Q(n)$, and we refer to their papers for details. The behaviour of $g(r)$ for large r is determined by the behaviour of the $Q(n)$ for large n. The asymptotic form $Q(n)\to 1-an^{-1}$ corresponds to a power law $g(r)\sim r^{-2a}$, and the asymptotic form $Q(n)\to 1-bn^{\theta-1}$, $0<\theta<1$, to the anomalous exponential decay $g(r)\sim \exp[-(r/\tilde{\xi})^{2\theta/(1+\theta)}]$, where $\tilde{\xi}=\{[\theta/(1+\theta)]^{1+\theta}b^{-1}\}^{1/2\theta}$.

To calculate the behaviour of $Q(n)$ for large n, we consider $K_i(m,n)$ which vary so slowly in m and n that the difference equations (4), (5) may be replaced by nonlinear first-order partial differential equations. In terms of the p_i rather than the K_i the differential equations are given by

$$\begin{aligned}\frac{\partial p_1}{\partial n}&=p_1^2\frac{\partial p_1}{\partial m}+[p_1(1-p_1^2)/p_2]\frac{\partial p_2}{\partial m}\\ \frac{\partial p_2}{\partial n}&=p_1p_2\frac{\partial p_1}{\partial m}-p_1^2\frac{\partial p_2}{\partial m}.\end{aligned}\tag{8}$$

Making the substitution $u=p_1/p_2$, $v=1/p_2$ and regarding m and n rather than u and v as the dependent variables, one is led to the linear equations

$$v\frac{\partial m}{\partial u}=-u\frac{\partial n}{\partial v}\qquad v\frac{\partial m}{\partial v}=-u\frac{\partial n}{\partial u}.\tag{9}$$

Equations (9) are to be solved with the boundary conditions $u(0,n)=0$ (which corresponds to $K_2(0,n)=0$ and $p_1(0,n)=0$; see figure 1) and $u(\infty,n)=u_B$, $v(\infty,n)=v_B$. In terms of the variables u, v the bulk criticality condition is $v_B-u_B=2$.

Apart from the minus signs in equation (9) and in the criticality condition, the flow equations in the variables u and v are the same as in the Ising case. Following in the footsteps of Hilhorst and van Leeuwen, we consider superpositions of separable solutions of the form

$$\begin{aligned} m(u, v) &= u \int_0^\infty \mathrm{d}\rho\, w(\rho) \exp(-\rho u_{\mathrm{B}}) I_1(\rho u)[K_1(\rho v_{\mathrm{B}}) I_0(\rho v) + I_1(\rho v_{\mathrm{B}}) K_0(\rho v)] \\ n(u, v) &= -v \int_0^\infty \mathrm{d}\rho\, w(\rho) \exp(-\rho u_{\mathrm{B}}) I_0(\rho u)[K_1(\rho v_{\mathrm{B}}) I_1(\rho v) - I_1(\rho v_{\mathrm{B}}) K_1(\rho v)] \end{aligned} \tag{10}$$

where the I_μ and K_μ are modified Bessel functions. $w(\rho)$ is a weight function which is chosen to match the initial system of interest for n fixed, $m \to \infty$. The choice $w(\rho) \to C\rho^{1/y+1/2}$ for $\rho \to \infty$ corresponds to inhomogeneous $K_i(m)$ of the form (3), with

$$A_1 = \tfrac{1}{2} K_{1\mathrm{B}}(1 - 2K_{1\mathrm{B}})A, \qquad A_2 = \tfrac{1}{8}(1 + 2K_{1\mathrm{B}})^2 A \tag{11}$$

$$A = \left[\left(\frac{2}{\pi}\, \frac{K_{1\mathrm{B}}(1 - 2K_{1\mathrm{B}})}{(1 + 6K_{1\mathrm{B}})^2}\right)^{1/2} C\Gamma(1/y)\right]^y. \tag{12}$$

To calculate the asymptotic behaviour of $Q(n)$ for large n, we consider (10) in the limit m fixed, $n \to \infty$, recalling that u and $\delta v = v - 2$ are small quantities near the surface and near criticality. Analysing the resulting form for $Q(n)$ as discussed following (7), we find that $g(r)$ decays according to (1) with $d = 2$ and $\nu = \frac{1}{2}$. For $y > 2$, $\eta_\parallel = 2$, and in the marginal case $y = 2$, $\eta_\parallel$ has the non-universal form

$$\eta_\parallel = 2 + 2\left(\frac{1 + 6K_{1\mathrm{B}}}{1 - 2K_{1\mathrm{B}}} A\right)^{1/2}. \tag{13}$$

The characteristic length $\tilde{\xi}$ for $y < 2$ is given by

$$\tilde{\xi} = [\tfrac{1}{2}(1 - \tfrac{1}{2}y)A^{-1/2}]^{2/(2-y)} \left[\left(\frac{1}{\pi}\, \frac{1 - 2K_{1\mathrm{B}}}{1 + 6K_{1\mathrm{B}}}\right)^{1/2} \frac{\Gamma(1/y)}{\Gamma(1/y + \frac{1}{2})}\right]^{y/(2-y)}. \tag{14}$$

This concludes our discussion of the correlation of the surface spins for the Gaussian model on a triangular lattice. The correlation function for internal spins and the magnetisation profile with a surface field may be calculated with the same differential real-space renormalisation technique, and we intend to consider these quantities in a future publication. The corresponding calculation for Ising spins is difficult if not impossible, since one must contend with triplet couplings generated by the star–triangle transformation, which, however, are absent in the Gaussian case.

The critical behaviour of the homogeneous Gaussian model is essentially independent of the dimension of the system, and one would expect the principal results obtained above ($\eta_\parallel = 2$ for $y > 2$, $\eta_\parallel$ non-universal for $y = 2$, anomalous exponential decay for $y < 2$) to hold for other dimensions besides 2. We have also considered a d-dimensional semi-infinite continuum Gaussian model (see Bray and Moore 1977, Cordery and Griffin 1981, and references therein) with the Hamiltonian

$$\frac{\mathcal{H}}{k_{\mathrm{B}}T} = \tfrac{1}{2} \int \mathrm{d}^d x [(\nabla s(\boldsymbol{x}))^2 + (t_{\mathrm{B}} + Az^{-y} + c\delta(z)) s(\boldsymbol{x})^2]. \tag{15}$$

Here $s(\boldsymbol{x})$ is the spin density at point $\boldsymbol{x} = (\boldsymbol{r}, z)$, with $\boldsymbol{r}$ and z parallel and perpendicular to the surface, respectively. The integration in (15) extends over the half-space $z > 0$. The surface interaction parameter c is assumed to be positive, corresponding to the 'ordinary' transition. The quantity $t_B + Az^{-y}$ is an inhomogeneous local temperature variable; $t_B = 0$ corresponds to the bulk critical temperature.

It is convenient to consider the Fourier component with wavevector k, $g_k(z, z')$, of the correlation function $\langle s(\boldsymbol{r}, z)s(\boldsymbol{r}', z')\rangle$, Fourier transformed in $\boldsymbol{r} - \boldsymbol{r}'$. This quantity satisfies the one-dimensional inhomogeneous 'Schrödinger' equation (Bray and Moore 1977)

$$\left(-\frac{d^2}{dz^2} + k^2 + t_B + Az^{-y} + c\delta(z)\right)g_k(z, z') = \delta(z - z'). \tag{16}$$

From (16) one sees that t_B, A and c transform as $t'_B = b^2 t_B$, $A' = b^{2-y}A$, $c' = bc$ as lengths are rescaled by b, consistent with the bulk exponent $\nu = \frac{1}{2}$ and the crossover exponents $\phi_A = 1 - \nu y$ (Burkhardt 1982a,b, Cordery 1982) and $\phi_c = 1 - \nu$ (Bray and Moore 1977). The temperature inhomogeneity is irrelevant for $y > 2$, which implies the same exponent $\eta_\parallel = 2$ as in the homogeneous semi-infinite case $A = 0$.

In the marginal case $y = 2$, $g_k(z, z')$ can be constructed explicitly (Bray and Moore 1977) from the two linearly independent solutions of the homogeneous differential equation corresponding to (16). These solutions have the form $\sqrt{z}I_\mu(\kappa z)$, $\sqrt{z}K_\mu(\kappa z)$, where I_μ and K_μ are modified Bessel functions, $\kappa = \sqrt{k^2 + t_B}$, and $A = \mu^2 - \frac{1}{4}$. $\eta_\parallel$, as pointed out by Cordery and Griffin (1981), is non-universal and depends continuously on A. An explicit expression for $\eta_\parallel$ may be found from the asymptotic behaviour $g_k(z, z') \sim k^{-1+\eta_\parallel} \sim k^{2\mu}$ for small k and $t_B = 0$, which implies

$$\eta_\parallel = 1 + \sqrt{1 + 4A}. \tag{17}$$

Non-universal quantities depend on the details of the model, and expressions (13) and (17) are similar but not identical.

For arbitrary $y < 2$ the $k = 0$ Fourier component $g_0(z, z')$ at the bulk critical temperature $t_B = 0$ can be constructed explicitly from the solutions $\sqrt{z}I_{\bar{\mu}}((z/\bar{\xi})^{1-y/2})$, $\sqrt{z}K_{\bar{\mu}}((z/\bar{\xi})^{1-y/2})$ to the homogeneous differential equation corresponding to (16) (see, for example, Schiff 1968). Here $\bar{\mu} = 1/(2 - y)$, and

$$\bar{\xi} = [(1 - \tfrac{1}{2}y)A^{-1/2}]^{2/(2-y)}. \tag{18}$$

From the asymptotic form of the Bessel functions for large arguments, one sees that $g_0(z, z')$ decays as $\exp[-(z/\bar{\xi})^{1-y/2}]$ for $z \gg z'$. This is an anomalous decay of the form (1) but perpendicular rather than parallel to the surface. Note the similarity between the correlation lengths $\tilde{\xi}$ and $\bar{\xi}$ in (14) and (18). One may conclude that the correlation function $\langle s(\boldsymbol{r}, z)s(\boldsymbol{r}', z')\rangle$ exhibits the same anomalous exponential decay perpendicular to the surface in the limit $z \gg z'$, $z \gg |\boldsymbol{r} - \boldsymbol{r}'|$ as $g_0(z, z')$ on the basis of a steepest-descent argument: Since $g_k(z, z')$, $k \neq 0$, falls off with an ordinary exponential decay $\exp(-kz)$, which is faster than the anomalous exponential decay, the $k = 0$ Fourier component in the Fourier integral for the correlation function in real space should outweigh the $k \neq 0$ components in the limit $z \gg z'$, $z \gg |\boldsymbol{r} - \boldsymbol{r}'|$. We have not yet succeeded in calculating the correlation function of the continuum model for $y < 2$ parallel to the surface, i.e. in the limit $|\boldsymbol{r} - \boldsymbol{r}'| \gg z, z'$.

In closing we note once again that the exact results of Hilhorst and van Leeuwen for the Ising model and our results for the Gaussian model are in complete agreement with the local scaling picture referred to in the paragraph containing equation (1), which predicts analogous behaviour in any semi-infinite system with interaction parameters which vary as $K(z) = K_B - Az^{-y}$ which has a divergent bulk correlation length.

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