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1983 J. Phys. A: Math. Gen. 16 L721

(http://iopscience.iop.org/0305-4470/16/18/008)

J. Phys. A: Math. Gen. **16** (1983) L721–L727. Printed in Great Britain

LETTER TO THE EDITOR

Real-space renormalisation of the smoothly inhomogeneous semi-infinite Ising model

Theodore W Burkhardt and Ihnsouk Guim
Department of Physics, Temple University, Philadelphia, Pa 19122, USA

Received 6 September 1983

Abstract. Using the Migdal–Kadanoff renormalisation method, we study the semi-infinite two-dimensional Ising model with inhomogeneous nearest-neighbour coupling constants that deviate from the bulk coupling by Am^{-y} for large m, m being the distance from the edge. The approximation correctly predicts irrelevance of the inhomogeneity for $y > \nu^{-1}$, a surface magnetic phase at the bulk critical temperature for $y < \nu^{-1}$, $A > 0$, and a non-universal A-dependent surface magnetic index in the marginal case $y = \nu^{-1}$.

Recent work (Hilhorst and van Leeuwen 1981, Blöte and Hilhorst 1983, Burkhardt and Guim 1983) has revealed a rich variety of surface critical behaviour in the semi-infinite Ising model with coupling constants that depend on the distance m from the surface. These papers consider nearest-neighbour couplings K_m, $m = 1, 2, \ldots$ (see figure 1) which approach the bulk coupling K_B as

$$K_m = K_B + Am^{-y}, \qquad m \gg 1 \tag{1}$$

for large m. We summarise some of the exact results.

(1) For $y > 1$ the inhomogeneity does not alter the universal surface critical behaviour. At bulk criticality the pair correlation function of the boundary spins, $g_{\|}(r)$, falls off as $r^{-\eta_{\|}}$, $\eta_{\|} = 1$, just as in the homogeneous semi-infinite case $A = 0$.

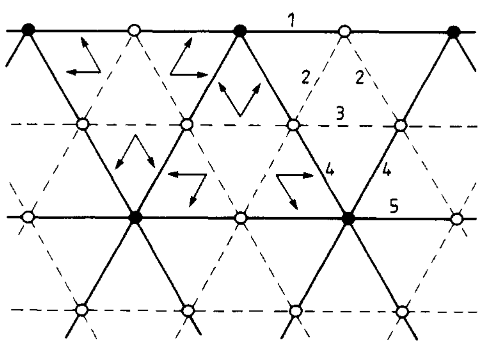

Figure 1. A portion of the semi-infinite triangular lattice. The numbers $m = 1, 2, \ldots$ label the bonds K_m in order of increasing distance from the edge. In the Migdal–Kadanoff renormalisation the broken bonds are moved onto the full bonds as indicated by arrows, with each broken bond shared equally by two full bonds. Then the spins represented by open circles are eliminated by decimation.

(2) For $y<1$ the surface critical behaviour is modified. At the bulk critical temperature there is a spontaneous boundary magnetisation m_1 in the case $A>0$ of stronger couplings near the surface. For either sign of A, $g_{\|}(r)$ decays according to the anomalous exponential form $\exp[-(r/\tilde{\xi})^{1-y}]$, $\tilde{\xi} \sim |A|^{-1/(1-y)}$ at bulk criticality.

(3) In the marginal case $y=1$ there is a spontaneous boundary magnetisation at the bulk critical temperature for A greater than a threshold value A_c. For $A<A_c$ and $A>A_c$, $g_{\|}(r)-g_{\|}(\infty) \sim r^{-\eta_{\|}(A)}$, with a non-universal exponent $\eta_{\|}(A)=|1-A/A_c|$. At $A=A_c$, $g_{\|}(r) \sim (\ln r)^{-1}$. For a more extensive discussion of the marginal case, see Blöte and Hilhorst (1983).

These results and analogous results for a smoothly inhomogeneous Gaussian model (Burkhardt and Guim 1982) are compatible with a local renormalisation picture applicable to any smoothly inhomogeneous system with a divergent bulk correlation length (Burkhardt 1982a, Cordery 1982). In this picture the bulk renormalisation transformation $K'=R(K)$ for the coupling constants of a homogeneous infinite system is replaced by

$$K'_m = R(K_{bm}), \qquad m \gg 1 \tag{2}$$

in the smoothly inhomogeneous semi-infinite case. Here b is the factor by which lengths are rescaled. Linearising (2) about the bulk fixed point K^*_B gives

$$K'_m - K^*_B = b^{y_t}(K_{bm}-K^*_B), \qquad m \gg 1 \tag{3}$$

where the scaling index y_t and the bulk exponent ν satisfy $y_t=\nu^{-1}$. Substituting $K'_m = K^*_B + A'm^{-y}$, $K_m = K^*_B + Am^{-y}$ into (3), one finds that A transforms according to

$$A' = b^{(1-\nu y)/\nu}A. \tag{4}$$

Equation (4) implies that the smooth inhomogeneity is a 'relevant' parameter (Fisher 1974) which modifies the critical behaviour for $y<\nu^{-1}$ but is 'irrelevant' for $y>\nu^{-1}$. A scaling analysis of the correlation function based on (4) indicates that the characteristic length $\tilde{\xi}$ in the correlation function $g_{\|}(r)$ for $y<\nu^{-1}$ diverges as

$$\tilde{\xi} \sim |A|^{-\nu/(1-\nu y)} \tag{5}$$

as $A \to 0$ at the bulk critical temperature (Burkhardt 1982a). A similar analysis of the boundary magnetisation m_1 gives

$$m_1 \sim A^{\beta_1/(1-\nu y)} \tag{6}$$

as $A \to 0$ from above (Burkhardt and Guim 1983). Here β_1 is the conventional surface exponent associated with the 'ordinary transition' (Binder 1983).

In this letter we carry out an approximate Migdal–Kadanoff real-space renormalisation (Kadanoff 1976, Burkhardt 1982b) of the smoothly inhomogeneous two-dimensional Ising model. The qualitative predictions of this simple approach agree nicely with many of the results mentioned above, and it provides a kind of insight which the exact calculations do not. Since the approximate renormalisation transformation has the form (2) for large m, it correctly predicts that the inhomogeneity of the couplings is relevant for $y<\nu^{-1}$ and irrelevant for $y>\nu^{-1}$. Knowing the explicit transformation for all values of m, we also obtain information which does not follow from the locality assumption (2) alone. In the marginal case $y=\nu^{-1}$ the approximate renormalisation does indeed yield an A-dependent surface magnetic index and a spontaneous magnetisation for A greater than a threshold value A_c.

Several authors (Švrakić and Wortis 1977, Burkhardt and Eisenriegler 1977, Dunfield and Noolandi 1980, Lipowsky and Wagner 1981, Nagai and Toyonaga 1981) have applied real-space renormalisation techniques to the homogeneous semi-infinite Ising model. In our work on smooth inhomogeneities, we begin with a semi-infinite triangular lattice of spins (figure 1), with bonds K_m, $m=1, 2, \ldots$ numbered in order of increasing distance from the edge. In the Migdal–Kadanoff renormalisation of the system, the broken bonds in figure 1 are moved onto the full bonds as indicated by arrows, with each broken bond shared equally by two full bonds. Then the spins represented as open circles are eliminated by decimation. The remaining spins, denoted by full circles, form a triangular lattice with twice the initial lattice constant. Using the same numbering scheme K'_m, $m=1, 2, \ldots$ for the renormalised coupling constants, we obtain the transformation

$$K'_1 = F(K_1 + \tfrac{1}{2}K_2, K_1 + \tfrac{1}{2}K_2) \tag{7}$$

$$K'_m = F(\tfrac{1}{2}K_{2m-2} + K_{2m-1} + \tfrac{1}{2}K_{2m}, \tfrac{1}{2}K_{2m-2} + K_{2m-1} + \tfrac{1}{2}K_{2m}), \qquad m = 3, 5, 7, \ldots \tag{8}$$

$$K'_m = F(\tfrac{3}{2}K_{2m-2} + \tfrac{1}{2}K_{2m-1}, \tfrac{1}{2}K_{2m-1} + \tfrac{3}{2}K_{2m}), \qquad m = 2, 4, 6, \ldots . \tag{9}$$

For Ising spins the function F is defined by

$$F(K_a, K_b) = \tanh^{-1}(\tanh K_a \tanh K_b). \tag{10}$$

Note that the transformation reduces to the form (2) for $m \gg 1$ in the case of K_m which vary sufficiently slowly with m. Thus the conclusions drawn from (2) apply. We shall see this more explicitly below.

In order to calculate the surface magnetic scaling index y_{h_1} (Binder 1983), one must generalise the renormalisation transformation to include a weak magnetic field h_1 applied to the boundary spins. Moving the bonds as described above (but not the local fields) and decimating, we obtain

$$h'_1 = \Lambda(K_1 + \tfrac{1}{2}K_2)h_1 + O(h_1^3) \tag{11}$$

where the function Λ is defined by

$$\Lambda(K) = (1 + \tanh K)^2/[1 + (\tanh K)^2]. \tag{12}$$

y_{h_1} is given by $y_{h_1} = \ln \Lambda(K_1^* + \tfrac{1}{2}K_2^*)/\ln 2$ at a fixed point of the transformation. A system with a spontaneous surface magnetisation is mapped onto a discontinuity fixed point (Nienhuis and Nauenberg 1975, Niemeijer and van Leeuwen 1976) with $K_1^* + \tfrac{1}{2}K_2^* = \infty$ and $y_{h_1} = d - 1 = 1$.

In the renormalisation transformation (7)–(9), all of the $K'_{m'}$ except K'_1 and K'_2 are determined by K_m with $m > m'$. Deep inside the system $m \approx 2m'$ as in (2). Thus, as the transformation equations are iterated, there is a flow of information about the interior toward the surface. It is the asymptotic form of K_m for large m which ultimately determines the fixed point onto which the system maps and hence the universality class. Since $K'_3, K'_4, \ldots$ are independent of K_1 and K_2, information about the semi-infinite nature of the system does not propagate into the interior on repeated renormalisation. This property, which is common to all the approximate real-space renormalisation groups for semi-infinite systems referenced above†, leads to difficulties in the calculation of the magnetisation profile (Burkhardt and Eisenriegler 1977).

† The method of Hilhorst and van Leeuwen (1981) is based on an exact mapping of the coupling constants with no change in the length scale. As the mapping is repeated, a surface-induced inhomogeneity does penetrate progressively deeper into the interior.

Equations (7)–(9) have a fixed point $K_1^* = 0.034$, $K_m^* = K_B^* = 0.305\,[0.275]$, $m = 2, 3, \ldots$ associated with the 'ordinary' transition of the homogeneous semi-infinite system. The number in brackets is the exact value $\frac{1}{4}\ln 3$ of the bulk critical coupling. For the thermal scaling index $y_t = \ln(\mathrm{d}F(2K_B^*, 2K_B^*)/\mathrm{d}K)/\ln 2$ and the surface magnetic scaling index y_{h_1}, one finds 0.747 [1] and 0.440 [$\frac{1}{2}$], respectively.

Small deviations of the coupling constants from the 'ordinary' fixed point may be expanded in terms of the right eigenvectors $\Psi_m^{(\alpha)}$ of the matrix $T_{mn} = \partial K'_m(K^*)/\partial K_n$ (Fisher 1974). With the corresponding eigenvalues written as 2^{y_α}, the eigenvectors satisfy

$$\Psi_1^{(\alpha)} = 2^{y_1 - y_\alpha}(\tfrac{1}{2}\Psi_1^{(\alpha)} + \tfrac{1}{4}\Psi_2^{(\alpha)}) \tag{13}$$

$$\Psi_m^{(\alpha)} = 2^{y_t - y_\alpha}(\tfrac{1}{4}\Psi_{2m-2}^{(\alpha)} + \tfrac{1}{2}\Psi_{2m-1}^{(\alpha)} + \tfrac{1}{4}\Psi_{2m}^{(\alpha)}), \qquad m = 3, 5, 7, \ldots \tag{14}$$

$$\Psi_m^{(\alpha)} = 2^{y_t - y_\alpha}(\tfrac{3}{8}\Psi_{2m-2}^{(\alpha)} + \tfrac{1}{4}\Psi_{2m-1}^{(\alpha)} + \tfrac{3}{8}\Psi_{2m}^{(\alpha)}), \qquad m = 2, 4, 6, \ldots \tag{15}$$

where $y_1 = -0.489$ in equation (13).

From the structure of equations (13)–(15), it follows that $\Psi_m^{(\alpha)}$ is completely determined once its behaviour for large m is specified. There are two irrelevant surface eigenvectors with $\Psi_m = 0$, $m > 2$. Apart from these, the only smoothly inhomogeneous solutions of (13)–(15) which do not diverge as $m \to \infty$ have the asymptotic form

$$\Psi_m^{(\mathrm{S})} \propto m^{-y}, \qquad m \text{ even or odd} \tag{16}$$

$$\Psi_m^{(\mathrm{NS})} \propto \begin{cases} -m^{-y}, & m \text{ even} \\ 2m^{-y}, & m \text{ odd} \end{cases} \tag{17}$$

where $y \geq 0$. The scaling indices $y_\alpha = y_{\mathrm{S}}(y)$, $y_{\mathrm{NS}}(y)$ corresponding to the symmetric and non-symmetric eigenvectors $\Psi_m^{(\mathrm{S})}$, $\Psi_m^{(\mathrm{NS})}$ are

$$y_{\mathrm{S}}(y) = y_t - y = (1 - \nu y)/\nu \tag{18}$$

$$y_{\mathrm{NS}}(y) = y_t - y - 2. \tag{19}$$

Since $y_t < 2$, $y_{\mathrm{NS}}(y)$ is negative, i.e. the non-symmetric eigenperturbation is irrelevant. In a system in which $K_m - K_B^* \propto \Psi_m^{(\mathrm{NS})}$, the compensating deviations of the even and odd couplings leave the system at bulk criticality, and the surface critical behaviour is 'ordinary'. The slope $\mathrm{d}K_{\mathrm{even}}/\mathrm{d}K_{\mathrm{odd}} = -\frac{1}{2}$, which follows from (17), is also implied by the exact critical surface.

We are particularly interested in coupling constants of the form (1), i.e. $K_m - K_B^* = A\Psi_m^{(\mathrm{S})}$. From (18) we see that A scales as in (4) and conclude once again that there is 'ordinary' surface critical behaviour for $y > \nu^{-1}$ and modified behaviour for $y < \nu^{-1}$.

Because of an inconsistency (Kadanoff 1976, Burkhardt 1982b) in the scaling of the correlation function under the Migdal–Kadanoff transformation, we have not attempted to calculate $g_\parallel(r)$ directly with the approximate renormalisation group. However, from (4) it is clear that the quantity $\tilde{\xi}(A) \propto |A|^{-\nu/(1-\nu y)}$ scales like a correlation length, i.e. $\tilde{\xi}(A') = b^{-1}\tilde{\xi}(A)$. Thus it is not surprising that the quantity appears as a characteristic length at the bulk critical temperature in the exact Ising results for $y < \nu^{-1}$.

In our approximate renormalisation scheme the boundary magnetisation per spin transforms as

$$m_1(K_1, K_2, \ldots) = \tfrac{1}{2}\Lambda(K_1 + \tfrac{1}{2}K_2)m_1(K'_1, K'_2, \ldots). \tag{20}$$

The transformation equations (7)–(9) map initial couplings of the form (1) with $y < \nu^{-1}$

and $K_B = K_B^*$ onto a weak-coupling fixed point with $K_m^* = 0$ for $A < 0$ and onto a strong-coupling fixed point with $K_m^* = \infty$ for $A > 0$. Thus for $y < \nu^{-1}$, $A > 0$ there is a spontaneous surface magnetisation at the bulk critical temperature. Equations (18) and (20) imply that the leading singular contribution to m_1 scales as $m_1(A) = 2^{y_{h_1}-d+1} m_1(2^{y_t - y} A)$. It follows that m_1 vanishes as $A^{\beta_1/(1-\nu y)}$ as $A \to 0$ in accordance with (6). Here $\beta_1 = (d-1-y_{h_1})/y_t$ is the conventional exponent of the ordinary transition (Binder 1983). The exact Ising result $m_1 \sim A^{1/[2(1-y)]}$ (Burkhardt and Guim 1983) is also consistent with (6).

We now turn to the marginal case $y = \nu^{-1}$. At bulk criticality, equations (7)–(9) map initial couplings of the form (1) with $y = \nu^{-1}$ onto an A-dependent fixed point $K_m^*(A)$, $m = 1, 2, \ldots$, i.e. a fixed line in the space of coupling constants. For large m, $K_m^*(A) = K_B^* + Am^{-y}$. We have determined $K_m^*(A)$ for smaller values of m by numerical iteration of the transformation equations. Results for four representative values of A are shown in figure 2. Each of the $K_m^*(A)$ increases monotonically with A. All of the $K_m^*(A)$ are finite for finite A except the surface coupling $K_1^*(A)$. From (7) one finds that $K_1^*(A)$ diverges (as $-\frac{1}{4}\ln(A_c - A)$) as A approaches the critical value A_c at which $K_2^*(A_c) = \ln 2$ from below. For $A > A_c$, $K_1^*(A) = \infty$.

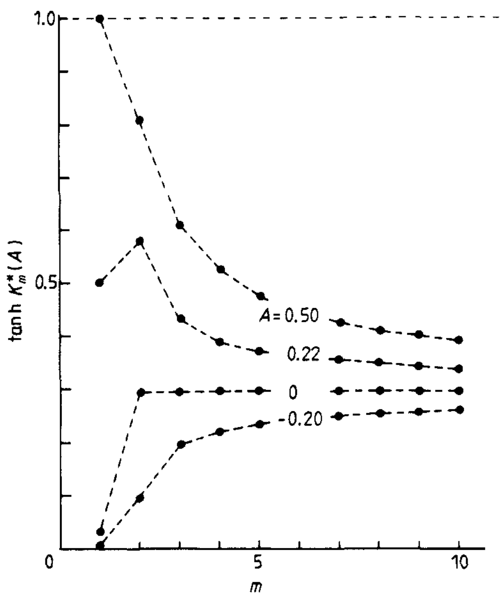

Figure 2. Fixed-point parameters $K_m^*(A)$ for four values of A in the marginal case $y = \nu^{-1}$. For $A > A_c = 0.237$, $K_1^*(A) = \infty$.

Since the fixed-point couplings $K_1^*(A)$, $K_2^*(A)$ vary with A, the scaling index y_{h_1}, calculated as described following equation (12), is non-universal. The full line in figure 3 shows the A dependence of y_{h_1} given by the approximate renormalisation group. For $A > A_c$, y_{h_1} has the value 1, which corresponds to a spontaneous surface magnetisation at the bulk critical temperature. The straight broken line indicates the exact Ising result, which follows from $\eta_\parallel = |1 - A/A_c|$ and the scaling relation $\eta_\parallel = d - 2y_{h_1}$ (Binder 1983). The exact value of A_c is $1/\sqrt{3} = 0.577$, whereas the approximate renormalisation group gives 0.237.

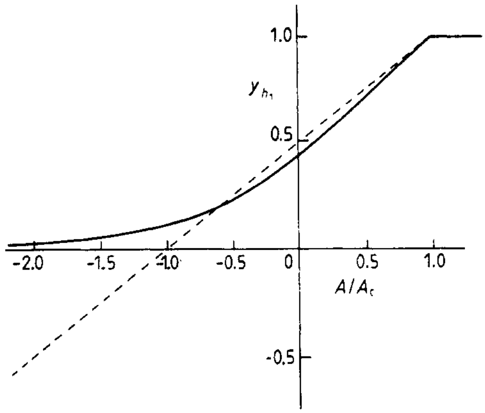

Figure 3. The non-universal surface magnetic index y_{h_1} as a function of A in the marginal case $y = \nu^{-1}$. The full line shows the prediction of the approximate renormalisation group. The straight broken line indicates the exact result. The approximate renormalisation group gives $\nu^{-1} = 0.747$, $A_c = 0.237$ in place of the exact values $\nu^{-1} = 1$, $A_c = 1/\sqrt{3} = 0.577$.

According to Blöte and Hilhorst (1983) and Burkhardt and Guim (1983), in the marginal case $y = \nu^{-1}$, m_1 disappears as $(A - A_c)^{1/2}$ as $A \to A_c$ from above at bulk criticality. We now consider the corresponding prediction of the approximate renormalisation group.

In terms of the variables $u = \tanh K_1$, $v = \tanh(\frac{1}{2}K_2)$, the transformation (7) for the surface coupling K_1 takes the form

$$u' = [(u+v)/(1+uv)]^2. \tag{21}$$

The fixed point $u^* = 1$ of (21) is attractive (corresponding to $K_1^*(A) = \infty$ in figure 2) for $v^*(A) \geq \frac{1}{3}$ (or $K_2^*(A) \geq \ln 2$). Near A_c, $v^*(A) = \frac{1}{3} + c(A - A_c)$, where c is a positive constant. Writing $u' = 1 - \delta u'$, $u = 1 - \delta u$, and $v = v^* + \delta v$ and linearising (21) for A near A_c gives

$$\delta u' = [1 - \tfrac{9}{4}c(A - A_c)]\, \delta u. \tag{22}$$

Equation (22) clearly reflects the change in stability of the fixed point $u^* = 1$ at $A = A_c$. Note that $\delta u'$ depends on δu but not on δv and the other couplings $K_3, K_4, \ldots$. For small δu (large K_1), $\Lambda(K_1 + \frac{1}{2}K_2) \to 2(1 - \frac{1}{16}(\delta u')^2)$. Thus (20) becomes

$$m_1(\delta u) = [1 - \tfrac{1}{16}(\delta u')^2] m_1(\delta u'). \tag{23}$$

Iterating (22) and (23) with the boundary condition $m_1(0) = 1$, one finds that m_1 vanishes as $\exp[-k/(A - A_c)]$ as $A \to A_c$ from above. Here k is a positive constant which depends on the initial value of δu.

Thus the approximate renormalisation group predicts that m_1 vanishes with an essential singularity at $A = A_c$ instead of the power law $m_1 \sim (A - A_c)^{1/2}$. There are other exact results for $y = \nu^{-1}$, $A > A_c$ for which we have found no simple explanation in terms of real-space renormalisation, for example, the non-universality of the exponent $\eta_\parallel$ and the asymmetry of the exponent $\nu_\parallel$ (Blöte and Hilhorst 1983).

Despite these shortcomings, the approximate renormalisation does capture the essential difference between the cases $y > \nu^{-1}$ and $y < \nu^{-1}$. The calculations described here served us as a valuable guide in formulating the scaling predictions (5) and (6).

The qualitative picture (see figure 2) which gives rise to the non-universality of y_{h_1} is independent of the details of the spin model and renormalisation procedure. Thus we expect A-dependent surface critical exponents to be a general property of smoothly inhomogeneous semi-infinite systems with $y = \nu^{-1}$. Exact results for the Gaussian model (Burkhardt and Guim 1982) support this view.

We thank K Binder, H J Hilhorst and J M J van Leeuwen for stimulating discussions. We appreciate the hospitality of the Institut für Festkörperforschung, Jülich, where this work was begun.

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