

Rapid note

Critical behaviour of three-dimensional Ising ferromagnets at imperfect surfaces: Bounds on the surface critical exponent β_1

H.W. Diehl

Fachbereich Physik, Universität - Gesamthochschule Essen, 45117 Essen, Germany

Received: 19 January 1998 / Revised: 27 January 1998 / Accepted: 28 January 1998

Abstract. The critical behaviour of three-dimensional semi-infinite Ising ferromagnets at planar surfaces with (i) random surface-bond disorder or (ii) a terrace of monatomic height and macroscopic size is considered. The Griffiths-Kelly-Sherman correlation inequalities are shown to impose constraints on the order-parameter density at the surface, which yield upper and lower bounds for the surface critical exponent β_1 . If the surface bonds do not exceed the threshold for supercritical enhancement of the pure system, these bounds force β_1 to take the value β_1^{ord} of the latter system's ordinary transition. This explains the robustness of β_1^{ord} to such surface imperfections observed in recent Monte Carlo simulations.

PACS. 68.35.Rh Phase transitions and critical phenomena – 75.10.Hk Classical spin models – 78.30.Ly Disordered solids

In a recent paper Pleimling and Selke (PS) [1] reported the results of a detailed Monte Carlo analysis of the effects of two types of surface imperfections on the surface critical behaviour of $d = 3$ dimensional semi-infinite Ising models with planar surfaces and ferromagnetic nearest-neighbour (NN) interactions: (i) random surface-bond disorder and (ii) a terrace of monatomic height and macroscopic size on the surface. For type (i), both the ordinary and special transitions were studied. They found that the asymptotic temperature dependence of the disorder-averaged surface magnetization on approaching the bulk critical temperature T_c from below could be represented by a power law $\sim |\tau|^{\beta_1}$ with $\tau \equiv (T - T_c)/T_c$, where β_1 agreed, within the available numerical accuracy, with the respective values $\beta_1^{\text{ord}} \simeq 0.8$ and $\beta_1^{\text{sp}} \simeq 0.2$ of the pure system's ordinary and special transitions. For type (ii), where the interaction constants were chosen such that only an ordinary transition could occur, the same value β_1^{ord} of the perfect system was found for β_1 .

Their findings for the case of (i) are in conformity with the relevance/irrelevance criteria of Diehl and Nüsser [2, 3] according to which the pure system's surface critical behaviour should be expected to be stable or unstable with respect to short-range correlated random surface-bond disorder depending on whether the surface specific heat C_{11} [4] of the pure system remains finite or diverges at the transition. It is fairly well established [5, 6] that C_{11} approaches a finite constant at the ordinary transition, but has a leading thermal singularity $\sim |\tau|^{(d-1)\nu-2\Phi}$ at the special transition, where Φ is the surface crossover

exponent. In the latter case, the condition for irrelevance, $\Phi < (d-1)\nu/2$, reduces to

$$\Phi < \nu \quad (1)$$

in $d = 3$ bulk dimensions. Since various Monte Carlo simulations [7–9] (though not all [10]) and renewed field-theory estimates [11] suggest a value of Φ between 0.5 and 0.6, definitely smaller than the accepted value 0.63 of ν for $d = 3$, one may be quite confident that the condition (1) holds. Thus short-range correlated surface-bond disorder should be irrelevant in the renormalization-group sense at both transitions.

Irrelevance criteria of the above Harris type [2, 3] seem to work quite well in practice. Yet, from a mathematical point of view, they are rather weak because they are nothing but a necessary (though not sufficient) condition for stability of the pure system's critical behaviour.

In this note, I shall employ the Griffiths-Kelly-Sherman (GKS) inequalities [12] to obtain upper and lower bounds on the surface magnetization densities of both types of imperfect systems, bounds that are given by surface magnetizations of analogous systems without such imperfections. Their known asymptotic temperature dependence near T_c will then be exploited to obtain restrictions on the surface critical behaviour of the imperfect systems considered. For some cases of interest studied by PS [1], the equality $\beta_1 = \beta_1^{\text{ord}}$ will be rigorously established.

Following these authors, let us consider an Ising model with ferromagnetic NN interactions on a simple cubic lattice of size $L_x \times L_y \times L_z$. Periodic boundary conditions

will be chosen along two principal axes (the x and y directions), and free boundary conditions along the third one (the z direction), so that the surface consists of the top layer at $z = 1$ and the bottom layer at $z = L_z$. Associated with each pair of spins on NN sites i and j is an interaction constant $J(i, j) > 0$, which we assume to have the same value J whenever i or j (or both) belong to layers with $1 < z < L_z$.

In the case of surface-bond disorder, which we consider first, the $J(i, j) \equiv J^{(s)}(i, j)$ of all NN pairs of surface sites are independent random variables. The probability density $P(J_1)$ of any one of these will be assumed to have support only in the interval $[J_1^<, J_1^>]$ (with $J_1^> > J_1^< > 0$). This is in conformity with, but less restrictive than, PS's assumption that J_1 takes just two values $J_1^<$ and $J_1^>$, either one with probability 1/2. We will also assume that all (bulk and surface) spins are exposed to the same magnetic field $H > 0$, whose limit $H \rightarrow 0^+$ will be taken after the thermodynamic limit has been performed.

Let $K \equiv J/k_B T$ and $h \equiv H/J$. Define $\mathbf{r}^{(s)}$ to be the set of all dimensionless surface coupling constants $J^{(s)}(i, j)/J$. Let $m(i; K, \mathbf{r}^{(s)}, h) \equiv \langle s_i \rangle$ be the thermal average of a spin at site i for a given disorder configuration $\mathbf{r}^{(s)}$, and denote the corresponding quantity of the perfect system with uniform NN surface coupling $J_1 = rJ$ as $m(i; K, r, h)$. Since all interactions are ferromagnetic, the GKS inequalities [12] are valid. Averages of products of spin variables are monotone non-decreasing functions of all variables $J(i, j)$ and H . Hence, for finite L_x, L_y , and L_z , $m(i; K, \mathbf{r}^{(s)}, h)$ is bounded by $m(i; K, r^<, h)$ from below and by $m(i; K, r^>, h)$ from above. We choose $i \equiv i_s$ to be a surface site, take the thermodynamic limit (first) and then let $H \rightarrow 0^+$. The bounds converge towards the respective values of $m_1(K, r, 0^+)$, the spontaneous magnetization of the surface layers per site, for $r = r^<$ and $r^>$. Thus we obtain

$$m_1(K, r^<, 0^+) \leq m(i_s; K, \mathbf{r}^{(s)}, 0^+) \leq m_1(K, r^>, 0^+). \quad (2)$$

The following limiting forms of m_1 are well established [1, 4, 7, 13, 14]:

$$m_1 = \begin{cases} C_1 |\tau|^{\beta_1^{\text{ord}}} [1 + o(\tau)] & \text{as } \tau \rightarrow 0^- \text{ at fixed } r < r_c, \\ C_1' |\tau|^{\beta_1^{\text{sp}}} [1 + o(\tau)] & \text{as } \tau \rightarrow 0^- \text{ at fixed } r = r_c, \\ m_{1c} + O(\tau) & \text{as } \tau \rightarrow 0^\pm \text{ at fixed } r > r_c, \end{cases} \quad (3)$$

where $r_c \simeq 1.50$ [7] is the critical value associated with the special transition. The quantities $m_{1c} > 0$, C_1 , and C_1' are nonuniversal, whence the first two depend on r .

Consider first the case $r^> < r_c$. Let $C^<$ and $C^>$ be the values of C_1 for $r = r^<$ and $r = r^>$, respectively. (These satisfy $0 < C^< \leq C^> < \infty$ provided $0 < J < \infty$ and $0 < J_1^< \leq J_1^> < \infty$.) It follows that there exists a number $\epsilon > 0$ independent of the disorder configuration $\mathbf{r}^{(s)}$ such that

$$C^> \leq m[i_s; K(\tau), \mathbf{r}^{(s)}, 0^+] |\tau|^{-\beta_1^{\text{ord}}} \leq C^< \quad (4)$$

whenever $-\epsilon < \tau < 0$. We denote the average of a quantity Q over all choices of the random variables $\mathbf{r}^{(s)}$ as \overline{Q} . Upon averaging $m(i_s; \cdot)$ to obtain the disorder-averaged surface magnetization $\overline{m_1}$, we see that the inequality (4) holds for $\overline{m_1} |\tau|^{-\beta_1^{\text{ord}}}$ as well. An elementary consequence is: If $\overline{m_1}$ has a well-defined critical exponent β_1^{dis} in the sense that [15]

$$\beta_1^{\text{dis}} = \lim_{\tau \rightarrow 0^-} \frac{\ln \overline{m_1}(\tau)}{\ln \tau} \quad (5)$$

exists, then we have

$$\beta_1^{\text{dis}} = \beta_1^{\text{ord}}. \quad (6)$$

Two further implications of (4) are worth mentioning. First, if a surface critical exponent $\tilde{\beta}_1^{\text{dis}}$ can be defined *via* the analog of (5) for the most probable value of $m(i_s; \cdot)$ [16], then it must have the same value β_1^{ord} . Second, the inequality (4) also rules out a limiting τ dependence of the form $\sim |\tau|^{\beta_1} |\ln |\tau||^\varphi$ (standard logarithmic corrections) for $\overline{m_1}$ and the most probable value of $m(i_s; \cdot)$.

Consider next the case $r^> = r_c$. Let us again make the assumption that the limit (5) or the analogous one defining $\tilde{\beta}_1^{\text{dis}}$ exist. Then the inequalities

$$\beta_1^{\text{sp}} \leq \beta_1^{\text{dis}} \leq \beta_1^{\text{ord}} \quad (7)$$

and their analogs for $\tilde{\beta}_1^{\text{dis}}$ can be deduced from (4) (*cf.* Lemma 3 of [15].)

The same reasoning applied in the case $r^> > r_c$ shows that β_1^{dis} or $\tilde{\beta}_1^{\text{dis}}$ must obey the relations

$$0 \leq \beta_1^{\text{dis}} \leq \beta_1^{\text{ord}} \quad (8)$$

whenever the limits (5) through which we defined them exist.

Likewise in the case $r^< = r_c$, the possible values of β_1^{dis} or $\tilde{\beta}_1^{\text{dis}}$ are restricted by

$$0 \leq \beta_1^{\text{dis}} \leq \beta_1^{\text{sp}} \quad (9)$$

at transitions at which $\overline{m_1}$ or the most probable value of $m(i_s; \cdot)$ [16] approach zero, respectively. On the other hand, it should be recalled that the surface critical exponent β_1^{ex} of the pure system's extraordinary transition requires a definition other than (5): One must subtract a regular background contribution m_1^{reg} from m_1 and define β_1^{ex} through the limiting behaviour $m_1 - m_1^{\text{reg}} \sim |\tau|^{\beta_1^{\text{ex}}}$. For transitions of the impure systems at which $\overline{m_1}$ approaches a constant $\neq 0$, it would also not make much sense to define β_1^{dis} *via* (5). Of course, for surface critical exponents β_1^{dis} not given by (5), the above bounds do *not* apply. This means that they cannot be utilized to draw conclusions about the surface critical exponent β_1^{ex} of the impure system's extraordinary transition. However, for a special transition of the impure system with $\overline{m_1}(\tau = 0) = 0$, the inequalities (9) hold.

The inequality (2) rules out that the impure system has an ordered surface phase for $T > T_c$ whenever $r^> \leq r_c$.

In order that the impure system can have an extraordinary or special transition, the distribution $P(J_1)$ of the surface couplings typically will have to extend beyond the critical-enhancement threshold $r_c J$ of the pure system. But even if $r^> > r_c$, an ordinary transition may still occur if the surface bonds ‘on average’ are not sufficiently enhanced (*cf.* [1]). However, if the support of $P(J_1)$ extends beyond $r_c J$, then disorder configurations for which macroscopically large surface regions have the same supercritical value ($> r_c J$) of J_1 occur with finite probability. This happens even if the impure system (for a typical realization of disorder) undergoes an ordinary transition, albeit with exponentially small probability. By analogy with the bulk case [17], I expect surface quantities like \overline{m}_1 and the disorder-averaged surface free energy to be *non-analytic* functions of the surface magnetic field H_1 at $H_1 = 0$ for temperatures between the bulk critical temperature T_c and the temperature $T_s(r^>) > T_c$ at which the semi-infinite pure system with homogeneous surface coupling $J_1 = r^> J$ undergoes a transition to a surface-ordered, bulk-disordered phase. That is, they should display *Griffiths singularities* [17], a problem on which we will not embark further here.

Turning now to the case of surfaces with a terrace, we start from a pure Ising model of the sort considered above. Just as PS, we assume that *all* NN couplings $J(i, j)$ (including those between surface sites) have the same value J . Let us denote thermal averages pertaining to this system by a superscript [I], writing, *e.g.*, $m^{[I]}(i; K) = \langle s_i \rangle^{[I]}$. We consider another system, [II], which differs from [I] through the addition of a zeroth layer at $z = 0$ whose spins are assumed to interact among themselves and with the spins in the $z = 1$ layer *via* NN interaction constants J_1 and J , respectively. To obtain a system with a terrace, [T], we choose a subregion of the zeroth layer (the terrace) and remove all those NN bonds J and J_1 that are connected to lattice sites of this layer outside the terrace region. PS considered a strip-like terrace of size $(L_x/2) \times L_y$, and assumed that $J_1 = J$. For our considerations, the precise form and size of the terrace region will not be important. (One could even assume that an arbitrary subset of the spins in the zeroth layer are decoupled from the rest of the system.)

Let i_1 be an arbitrary lattice site in the $z = 1$ layer. Since the systems [I], [T], and [II] differ by the addition of ferromagnetic interactions, we have from the GKS inequalities,

$$m^{[I]}(i_1; K, h) \leq m^{[T]}(i_1; K, r, h) \leq m^{[II]}(i_1; K, r, h) \quad (10)$$

where, as before, $h = H/J > 0$ is a uniform magnetic field and $r = J_1/J$. In the thermodynamic limit $L_x, L_y, L_z \rightarrow \infty$, the lower and upper bounds converge towards $m_1(K, h)$, the magnetization per site of the topmost layer, and to $m_2(K, r, h)$, the magnetization per site of the layer underneath the topmost layer, respectively. If we assume that $r < r_c$ (subcritical surface enhancement) and take the limit $h \rightarrow 0^+$, then the limiting form shown in the first line of (3) applies to both m_1 and m_2 (with different values of C_1). As a straightforward consequence we find that

the surface critical exponent β_1 of $m^{[T]}(i_1; K, r, 0^+)$ (for an arbitrary site i_1 with $z = 0$) strictly satisfies $\beta_1 = \beta_1^{\text{ord}}$.

It is evident that the same reasoning can be applied to the analogous two-dimensional model with a terrace to conclude that β_1 takes the exactly known value $\beta_1^{\text{ord}} = 1/2$. Likewise, the inequality (4) and the result (6) carry over to the two-dimensional case, giving $\beta_1^{\text{dis}} = 1/2$ for all values of $r < \infty$, since $r_c = \infty$ for $d = 2$. Note also that the inequality (4) excludes the possibility of an asymptotic temperature dependence of the form $\overline{m}_1 \approx \text{const} |\tau|^{1/2} |\ln |\tau||^p$ (*i.e.*, of logarithmic correction factors). This is because it is known for the pure case that no such logarithmic corrections appear in the limiting form of m_1 .

Results of Monte Carlo simulations on the surface critical behaviour of two-dimensional Ising models with bond disorder have been reported in two recent papers [18]. However, in this work random bond disorder was assumed to be present both in the bulk and at the surface, a case not captured by our reasoning. Nevertheless, \overline{m}_1 was found to behave as $|\tau|^{1/2}$, apparently without logarithmic corrections, even though the presence of such a correction could be detected in the limiting form of the disorder-averaged bulk order parameter.

I am indebted to W. Selke for informing me about the work [1] prior to publication, and to him, Joachim Krug, and Kay Wiese for a critical reading of the manuscript. This work has been supported by the Deutsche Forschungsgemeinschaft through the Leibniz program.

References

1. M. Pleimling, W. Selke, *Eur. Phys. J. B* **1**, 385 (1998).
2. H.W. Diehl, A. Nüsser, *Z. Phys. B* **79**, 69 (1990).
3. These criteria are of a similar nature as the familiar Harris criterion, which assesses the relevance or irrelevance of random bond bulk disorder; see A.B. Harris, *J. Phys. C* **7**, 1671 (1974).
4. For background on surface critical behaviour, see H.W. Diehl, in *Phase Transitions and Critical Phenomena*, edited by C. Domb, J.L. Lebowitz (Academic Press, London, 1986), Vol. 10, pp. 75–267; K. Binder, in *Phase Transitions and Critical Phenomena*, edited by C. Domb, J.L. Lebowitz (Academic, London, 1983), Vol. 8, pp. 1-144; H.W. Diehl, *Int. J. Mod. Phys. B* **11**, 3593 (1997), preprint cond-mat/9610143.
5. S. Dietrich, H.W. Diehl, *Z. Phys. B* **51**, 343 (1983).
6. H.W. Diehl, S. Dietrich, E. Eisenriegler, *Phys. Rev. B* **27**, 2937 (1983).
7. D.P. Landau, K. Binder, *Phys. Rev. B* **41**, 4633 (1990).
8. C. Ruge, S. Dunkelmann, F. Wagner, *Phys. Rev. Lett.* **69**, 2465 (1992).
9. C. Ruge, S. Dunkelmann, F. Wagner, J. Wulf, *J. Stat. Phys.* **73**, 293 (1992).
10. M. Vendruscolo, M. Rovere, A. Fasolino, *Europhys. Lett.* **20**, 547 (1992).
11. H.W. Diehl, M. Shpot, *Phys. Rev. Lett.* **73**, 3431 (1994), and to be published.
12. R.B. Griffiths, *J. Math. Phys.* **8**, 478 (1967); D.G. Kelly, S. Sherman, *J. Math. Phys.* **9**, 466 (1968).

13. To my knowledge, not all aspects of these limiting forms have been proven in a mathematically rigorous fashion, but they are consistent with all known results. For rigorous results on the 3D semi-infinite Ising model, see J. Fröhlich, C.-E. Pfister, *Commun. Math. Phys.* **109**, 493 (1987); C.-E. Pfister, O. Penrose, *Commun. Math. Phys.* **115**, 691 (1988).
14. T.W. Burkhardt, H.W. Diehl, *Phys. Rev. B* **50**, 3894 (1994).
15. Cf. H.E. Stanley, *Introduction to Phase Transitions and Critical Phenomena, International series of monographs on physics* (Oxford University Press, Oxford, 1971), Eq. (3.2); note also that its Lemma 3 could be utilized to derive the result (6) from (4).
16. Quantities like $m_1 \equiv \sum_{i_s} \langle s_{i_s} \rangle / \sum_{i_s} 1$, the total magnetization of the surface per spin, may be expected to be self-averaging in the thermodynamic limit. Hence the value m_1 takes for any choice of the random variables $\mathbf{r}^{(s)}$ that occurs with reasonable probability should agree with $\overline{m_1}$. Once one accepts this, the distinction between β_1^{dis} and $\tilde{\beta}_1^{\text{dis}}$ becomes unnecessary. It is made here because the assumption of self-averaging is neither required nor used in the derivation of the given inequalities, and not to suggest a possible breakdown of self-averaging.
17. R.B. Griffiths, *Phys. Rev. Lett.* **23**, 17 (1969).
18. W. Selke, F. Szalma, P. Lajkó, F. Iglói, *J. Stat. Phys.* **89**, 1079 (1997); F. Iglói, P. Lajkó, W. Selke, F. Szalma, preprint cond-mat/9711182.