[2]P. W. Anderson, Phys. Rev. 124, 41 (1961).
[3]For a general review see *Magnetism*, edited by H. Suhl (Academic, New York, 1973), Vol. V.
[4]L. L. Hirst, Phys. Kondens. Mater. 11, 255 (1970); L. L. Hirst, in *Magnetism and Magnetic Materials—1974*, AIP Conference Proceedings No. 24, edited by C. D. Graham, Jr., G. H. Lauder, and J. J. Rhyne (American Institute of Physics, New York, 1975), p. 11.
[5]E. Boucai, B. Lecoanet, J. Pilon, J. L. Tholence, and R. Tournier, Phys. Rev. B 3, 3834 (1971).
[6]J. Gardner, to be published; see also H. J. Guntherodt and H. A. Meier, Phys. Kondens. Mater. 16, 25 (1973).
[7]A. Narath and D. C. Barham, Phys. Rev. B 7, 2195 (1973).
[8]B. Caroli, P. Lederer, and D. Saint-James, Phys. Rev. Lett. 23, 700 (1969).
[9]L. Dworin and A. Narath, Phys. Rev. Lett. 25, 1287 (1970).
[10]See also the extension of the Anderson model developed by Malmström and C. Blomberg, J. Phys. F 5, 1197 (1975).
[11]A. Narath, Phys. Rev. B 13, 3724 (1976).
[12]R. J. Holliday and W. Weyhmann, Phys. Rev. Lett. 25, 243 (1970).
[13]L. Dworin, Phys. Rev. Lett. 26, 1372 (1971).
[14]H. Shiba, Prog. Theor. Phys. 54, 967 (1975).
[15]R. Dupree and W. W. Warren, Jr., to be published.
[16]Even a substantial d-spin hyperfine field would have only a minor effect on our results.
[17]Shift results reported in Ref. 7 at 120 and 300 K have subsequently been identified as spurious; further efforts to observe the ^{59}Co NMR in this range of temperature have proved fruitless. A. Narath, private communication.
[18]We note that the complementary case *Au*V^{2+} (d^3) must have the opposite sign of Δ. From the contrast in behavior between these systems [see A. Narath and A. C. Gossard, Phys. Rev. 183, 391 (1969)] it is clear that the sign taken for Δ is correct.
[19]K. D. Schotte and U. Schotte, Phys. Rev. B 4, 2228 (1971).
[20]W. Götze and P. Schlottmann, J. Low Temp. Phys. 16, 87 (1974).
[21]G. Andersson, Acta Chem. Scand. 10, 623 (1956).
[22]Y. Yafet, J. Phys. Chem. Solids 30, 1957 (1969).
[23]A. Freeman and R. Watson, in *Magnetism*, edited by G. Rado and H. Suhl (Academic, New York, 1965), Vol. IIA.
[24]Analysis of a similar case is given by R. E. Walstedt and A. Narath, Phys. Rev. B 6, 4118 (1972).

COMMENTS

Exponent Inequalities at the Roughening Transition

Robert H. Swendsen*
Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-517 Jülich, Germany
(Received 30 July 1976)

The exponents describing the divergence of various measures of the width of an interface between two phases in an Ising ferromagnet at the roughening transition are shown to satisfy a set of rigorous inequalities.

In this Letter, I derive a set of inequalities for the roughening transition in an interface between two phases in an Ising ferromagnet.[1] The roughening transition is characterized by the divergence of various measures of the interface width at a temperature, T_R, below the bulk critical temperature, T_c, and is of great interest in the theory of crystal growth.[1,2] The inequalities that I present are useful in checking calculations of interface properties and, in particular, show that the published values of the roughening exponents obtained from low-temperature expansions are not self-consistent.[3,4]

I consider a three-dimensional (3D) Ising ferromagnet with (not necessarily isotropic) nearest-neighbor exchange. A 2D interface perpendicular to the z axis is imposed by some appropriate boundary conditions (antiperiodic in the z direction, for example) and the concentration of up spins in the nth layer (x-y plane) is denoted by $c_n \in [0, 1]$. For sufficiently low temperatures, the interface is localized[5,6] and the layer magnetization, $2c_n - 1$, takes on positive values on one side of the interface and negative values on the other. One can number the layers so that $c_n > \frac{1}{2}$ for $n \leq 0$ and $c_n < \frac{1}{2}$ for $n \geq 1$. Far from the interface, the magnetization takes on its bulk value, $\sigma = c_{-\infty} - c_{\infty}$.

We are primarily interested in the measures of the interface width given by the absolute moments

$$\langle |n|^k \rangle = \sum_{n=-\infty}^{\infty} |n|^k (c_n - c_{n+1}). \tag{1}$$

Since van Beijeren[6] has proven that

$$(c_{n-1}-c_n) \geqslant (c_n - c_{n+1}) \qquad (2)$$

for $n \geqslant 1$, we have $(c_n - c_{n+1}) \geqslant 0$ for all n from boundedness and the symmetry $c_{1-n} = 1 - c_n$. For $k \geqslant 1$, this gives $\langle |n|^k \rangle \leqslant \langle |n|^{k+1} \rangle$. If one defines T_k as the temperature at which $\langle |n|^k \rangle$ diverges, one has

$$T_k \geqslant T_{k+1}. \qquad (3)$$

If, on the other hand, all moments diverge at a single roughening temperature, T_R, with power laws of the form

$$\langle |n|^k \rangle \sim (T_R - T)^{-\theta_k}, \qquad (4)$$

one can derive a set of inequalities for the roughening exponents. For this purpose, I define the normalized absolute moments $\beta_k = \langle |n|^k \rangle / \sigma$. Noting that $(c_n - c_{n+1})/\sigma$ is non-negative and $\beta_0 = 1$, one can immediately write down the Lapunov inequalities[7,8]

$$\beta_k^{1/k} \leqslant \beta_{k+1}^{1/k+1} \qquad (5)$$

for positive integers k. Using Eq. (4), one finds the roughening-exponent inequalities

$$\theta_k / k \leqslant \theta_{k+1}/(k+1) \qquad (6)$$

since the bulk magnetization, σ, is bounded.

One can also extend the analysis to a local measure of the width, $M = 1/(c_0 - c_1)$. Using inequality (2), I first write down the series of inequalities

$$\langle |n| \rangle = 2\sum_{n=1}^{\infty} n(c_n - c_{n+1}) \geqslant 2(m+1)\sum_{n=m+1}^{\infty}(c_n - c_{n+1}) + 2\sum_{n=1}^{m} n(c_n - c_{n+1})$$
$$\geqslant (m+1)[\sigma - (c_0 - c_1)] - 2\sum_{n=1}^{m}(m+1-n)(c_1 - c_2), \qquad (7)$$

which is valid for all m. If one chooses $m = [\sigma - (c_0 - c_1)]/2(c_1 - c_2) - \delta$, where $\delta \in [0,1)$, thus ensuring that m is an integer, one finds

$$\langle |n| \rangle \geqslant M(\sigma - 1/M)^2/4. \qquad (8)$$

If M diverges at a temperature $T_M < T_c$, one has

$$T_M \geqslant T_1, \qquad (9)$$

since σ remains nonzero as $M \to \infty$.

If there is only a single roughening temperature, $T_R < T_c$, and M diverges with an exponent θ_M, one finds that

$$\theta_1 \geqslant \theta_M. \qquad (10)$$

Weeks, Gilmer, and Leamy[3] have calculated the exact values of the first eight coefficients in the low-temperature expansions of $\langle n^2 \rangle$, $\langle n^4 \rangle$, and M for an isotropic Ising ferromagnet. The apparent convergence of these series is good and becomes quite impressive if the original analysis is extended with an Euler transform[9] to reduce the influence of singularities near the negative real axis. The temperatures at which the Padé and Neville tables predict a divergence are $k_B T_M = 2.46$ J, $k_B T_2 = 2.60$ J, and $k_B T_4 = 2.64$ J. These values fail to satisfy inequalities (3) and (9). Furthermore, if one follows Weeks, Gilmer, and Leamy[3] in interpreting the calculated exponents ($\theta_M = 0.78$, $\theta_2 = 1.00$, $\theta_4 = 1.43$) as estimates of the roughening exponents at a single temperature, one finds that they violate inequalities (6) and (10). Attempts to calculate biased estimates[9] of the exponents using a single value of the roughening temperature give poor convergence and even more severe violations of the exponent inequalities.

Leamy, Gilmer, and Jackson[4] have presented the corresponding series for the solid-on-solid model (which is the limit of infinitely strong anisotropy).[1-4] They find $k_B T_M = 2.4904$ J and $k_B T_2 = 2.5568$ J, which fail to satisfy the inequalities by 2.6%. The apparently good convergence also led them to give the roughening exponents to three significant digits ($\theta_M = 0.972$ and $\theta_2 = 0.968$), but they violate the exponent inequalities by more than a factor of 2.[10]

The exact inequalities make it clear that the apparent regularity of the available terms in the low-temperature series is not characteristic of their asymptotic behavior and cannot be regarded as a demonstration of the existence of roughening.

I would like to thank Dr. H. Müller-Krumbhaar for helpful comments.

*Present address: Brookhaven National Laboratory, Upton, N. Y. 11917.

[1]W. K. Burton and N. Cabrera, Disc. Faraday Soc. 5, 33 (1949).

[2]W. K. Burton, N. Cabrera, and F. C. Frank, Philos. Trans. Roy. Soc. London. 243, 299 (1951).

[3]J. D. Weeks. G. H. Gilmer, and H. J. Leamy, Phys. Rev. Lett. 31, 549 (1973).

[4]H. J. Leamy, G. H. Gilmer, and K. A. Jackson, in *Surface Physics of Crystalline Materials*, edited by J. M. Blakely (Academic, New York, 1976).

[5]R. I. Dobrushin, Theory Probab. Its Appl. (USSR) 17, 619 (1972).

[6]H. van Beijeren, Commun. Math. Phys. 40, 1 (1975).

[7]A. M. Lapunov, Bull. Acad. Sci. St. Petersburg 13, 359 (1900).

[8]M. S. Fisz, *Probability Theory and Mathematical Statistics* (Wiley, New York, 1963), 3rd ed., p. 76.

[9]D. L. Hunter and G. A. Baker, Jr., Phys. Rev. B 7, 3346, 3377 (1973).

[10]The exponents recently calculated in a mean-field (MF) theory of roughening satisfy inequalities (6) and (10) as equalities. ($\theta_M{}^{MF}=\frac{1}{2}$, $\theta_2{}^{MF}=1$, $\theta_4{}^{MF}=2$.) R. H. Swendsen, Phys. Rev. B 15, 689 (1976).

ERRATA

PERHAPS A STABLE DIHYPERON. R. L. Jaffe [Phys. Rev. Lett. 38, 195 (1977)].

The flavor-octet dihyperon with $Y=1=0$ and $J^P=1^+$, H^*, does not couple to $\Lambda\Lambda$ or $\Sigma\Sigma$ because of statistics. It may be seen as a bump in $N\Xi$ invariant-mass plots or in the missing mass in $pp\rightarrow K^+K^+X$. (We thank Dr. L. Littenburg for calling this to our attention.)

The masses of the $J=2$ $\underline{8}$ and $\underline{27}$ were inadvertently omitted from Table I; they are 2066 and 2357 MeV, respectively, in the limit $m_s=0$.

SEARCH WITH SYNCHROTRON RADIATION FOR SUPERHEAVY ELEMENTS IN GIANT-HALO INCLUSIONS. C. J. Sparks, Jr., S. Raman, H. L. Yakel, R. V. Gentry, and M. O. Krause [Phys. Rev. Lett. 38, 205 (1977)].

On page 206, column 2, the sixteenth line from the top, the sentence should read, "The numerical values used for σ_i in units of 10^{-21} cm^2/atom are 2.22 for Cd $K\alpha$, 3.66 for Cs $K\alpha$, 0.24 for Th $L\gamma_{1,2,3}$, and 4.0 for $L\alpha_1$ of element 126 at 37 keV."