Axial next-nearest-neighbor Ising-model roughening transitions

Arjun Berera*
Department of Physics, University of California, Berkeley, Berkeley, California 94720

Byungnam Kahng
Department of Physics, Kun Kook University, Seoul 133, Korea
(Received 7 August 1992)

Low-temperature expansions are presented for the surface tension and second moment of the density gradient in the three-dimensional axial next-nearest-neighbor Ising model. Padé approximants for the second moment of the density gradient show a definite line of singularities in the space of coupling parameters. The surface tension is shown to be positive along this line. We conclude that our low-temperature expansion is internally consistent to seventh order, that the singularity structure we found is an exact property of the system, and that it is the roughening transition.

PACS number(s): 05.50.+q, 68.10.Cr

I. INTRODUCTION

The roughening transition is a type of two-dimensional thermodynamical singular behavior in the Kosterlitz-Thouless-universality class which occurs in many three-dimensional systems which have an interface. In mathematical terms this is a continuous transition characterized by a correlation length ξ which behaves as

$$\xi = e^{b(|T-T_R|^{1/2})/(T_R)} ,$$

For $T<T_R$. This contrasts the case of a second-order phase transition where $\xi=|T-T_c|^{-\nu}$. Another distinct feature of the roughening transition is the persistence of a divergent correlation length for $T>T_R$. Such behavior can be observed experimentally, for example, in a separated two-fluid solution through measurements of interfacial reflexivity.

In the context of the three-dimensional Ising model, the condition needed for a roughening transition to occur is the presence of an interface separating bulk regions of plus and minus spins at low temperature. As the temperature is increased the long-wavelength modes along the interface steadily become the dominant contribution to the surface free energy. This in turn implies that the spins along the planes next to the interface feel a uniform effect over the entire two-dimensional region. Furthermore the couplings that are perpendicular to the interface are small at low temperature and vanish at absolute zero as a simple spin-flip calculation can show. This implies that the effective perpendicular mean field is small. As such a coherent disordering of the bulk spins near the interface occurs and manifests observably as a wandering of the interface.

It was Weeks, Gilmer, and Leamy [1] who first obtained the roughening critical temperature in the three-dimensional Ising model using low-temperature expansion and Padé approximant methods. Recently, Kahng, Berera, and Dawson [2] and Berera and Kahng [3] have found the same transition in the Widom model [4]. Prompted by these results, we will explore the same behavior in the three-dimensional axial next-nearest-neighbor Ising (ANNNI) model. In this paper we will obtain, for the interface between two ferromagnetic phases of opposite spin of the ANNNI model, the low-temperature expansion to seventh order for the second moment of the density gradient and the surface tension. We will then compute the roughening transition line using d log Padé approximants for the second moment of the density gradient.

Before proceeding let us briefly review the ANNNI model. This lattice model has had a long history of use in the study of alloys, magnetic order, and various properties of real material (for a review of the ANNNI model see Ref. [4]). In years to come it may be replaced to a large extent by the Widom model [5], which has the attractive feature of isotropic, in addition to competing, microscopic interactions. However, at present much understanding about magnetic and alloy systems as well as extensive theoretical analysis of competing interactions has been studied in the context of the ANNNI model. Thus rigorous results such as low-temperature analysis about this model will remain useful for sometime both for theoretical and practical purposes.

In this respect there is another use for the work to be presented here. Up to now most applications using low-temperature expansions of the ANNNI model have relied on idealized bulk quantities. However, in many practical cases, real materials have large domains of bulk phase separated by interfaces. For these cases it would be beneficial to have precise knowledge about the interfacial properties and our calculations here serve this dual purpose of providing nontrivial high-order expansions of relevant interfacial quantities.

II. CALCULATION AND RESULTS

To proceed with the calculation, the Hamiltonian for the ANNNI model which we will use is

$$H=-\frac{1}{2}\sum_{i}\left[J_0\sum_{j=1}^{4}\sigma_i\sigma_{i+e_j^{xy}}+\alpha J_0\sum_{j=1}^{2}\sigma_i\sigma_{i+e_j^{z}}+J_2\sum_{j=1}^{2}\sigma_i\sigma_{i+e_j^{zz}}\right], \tag{1}$$

where the index i runs over all sites on the lattice, $\{e^{xy}\}$ are a set of four unit vectors along the axis in the xy plane, $\{e^{z}\}$ are a et of two unit vectors along the z direction, and $\{e^{zz}\}$ are a set of two vectors of length 2 along the z direction. The calculations presented in this paper will be for $\alpha=1$, for which the phase diagram obtained from Ref. [4] is shown in Fig. 1.

The low-temperature expansions that we have performed are defined in the two-dimensional parameter space of J_0 and J_2, restricted to the region of the bulk ferromagnetic phase. To facilitate the calculations, we define the parameter of smallness as

$$y\equiv e^{-4j_0}\ . \tag{2a}$$

In addition, we define another auxiliary parameter,

$$x\equiv e^{-4j_2}\ , \tag{2b}$$

where

$$j_0\equiv\frac{J_0}{kT} \tag{3a}$$

and

$$j_2\equiv\frac{J_2}{kT}\ . \tag{3b}$$

Note that the parameter x is not necessarily meant to be small but is introduced only as a notational convenience. Within this two-dimensional parameter space we will be looking for singular behavior along a one-dimensional slice. Our procedure will be to fix x and examine singular behavior along the y direction using Padé approximants.

In order to calculate the roughening line, we examine the low-temperature expansion of the second moment of the density gradient, $d\rho/dz$, defined on a discrete lattice as

$$\langle z^2\rangle=\sum_{z=-\infty}^{\infty}[\rho(z-\tfrac{1}{2})-\rho(z+\tfrac{1}{2})]z^2\ . \tag{4}$$

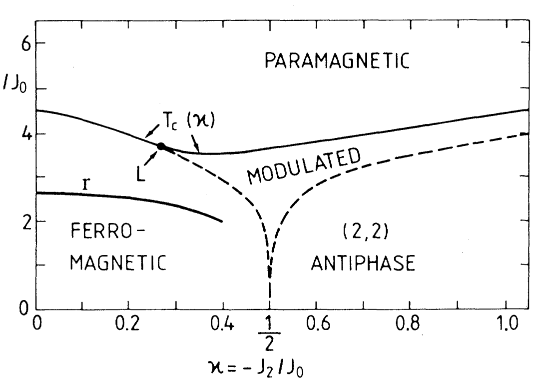

FIG. 1. Phase diagram obtained from Ref. [4] for the ANNNI model at $\alpha=1$. A sketch of the roughening line is denoted by r.

Observe that this quantity gives a measure of the square of the interfacial width. At low temperatures it will be finite, but at the roughening critical point it is expected to diverge with dominant singularity,

$$y^2(y-y_{R_x})^{-\Theta_{R_x}}\ , \tag{5}$$

where y_{R_x} is y as defined in Eq. (2a), evaluated at the roughening critical temperature, T_{R_x}, and Θ_{R_x} is the roughening critical exponent.

To confirm the validity of the roughening line it is also necessary to establish the positivity of the surface tension along the line. To clarify this point, let us take note that the roughening line we will obtain is based on a low-order series expansion and not the complete partition function. One must therefore be conservative about extracting information on singularity structure from such an approach especially when qualitative familiarity is lacking as is the case for the relatively unexplored roughening transition. As a reasonable check one can establish internal consistency within the order of expansion of the low-temperature series. To do this it is simplest to compute the surface tension since this quantity has readily identifiable and familiar qualitative features. Given that the surface tension computed to the same order is found to be positive, one can assume with good confidence that the singularity found from the series (A1) is associated with true physical attributes of the system and is not an artifact of a low-order series.

Turning to the results, our low-temperature expansions are to seventh order in y for $\langle z^2\rangle$ and surface tension Σ and are given in Appendix Eqs. (A1) and (A2), respectively. Observe that in the limit $J_2=0.0$, or equivalently $x=1$ (A1) agrees with the results in Ref. [1] and (A2) is the series for the surface tension of the three-dimensional Ising model as given in Ref. [6]. Both series in the Appendix have general applicability in the low-temperature ferromagnetic regime, although in the present work, we will study them only in the context of the roughening transition.

To compute the coefficients, a modified Martin type algorithm [2,3,7] was used to obtain all connected clusters and clusters with only one disconnected monomer. The remaining clusters were computed by hand. Our algorithm can incorporate summing over any general set of local interactions such as nearest and next-nearest couplings in the case of the ANNNI model and this plus diagonal couplings for the Widom model [2,3]. As such it is more elaborate than the original Martin algorithm for the nearest-neighbor Ising model. The extension to even higher orders in the low-temperature expansion is mainly hindered by the difficulty of counting the terms done by hand.

The numerical results of our low-temperature analysis are summarized in Table I. The first two columns give the coordinates of the roughening line that we found in terms of the parameters x and y. This was obtained by a Padé analysis [1] of the logarithmic derivative of the series (A1) (i.e., d log Padé analysis). Columns 3 and 4

TABLE I. Numerical results based on the low-temperature expansion series in the Appendix. Columns 1–5 were obtained by Padé analysis of the logarithmic derivative of series (A1). Column 6 was obtained by direct evaluation of series (A2).

x_R	y_R	j_{1R}	j_{2R}	Θ_R	Σ_R
0.698	0.214	0.386	0.09	0.876	0.967
0.787	0.214	0.386	0.06	0.906	0.851
0.887	0.214	0.385	0.03	0.947	0.734
1.000	0.214	0.385	0.00	0.997	0.619
1.128	0.214	0.386	−0.03	1.046	0.508
1.271	0.212	0.388	−0.06	1.074	0.407
1.433	0.205	0.396	−0.09	1.050	0.319
1.616	0.194	0.410	−0.12	0.947	0.249
1.822	0.178	0.431	−0.15	0.758	0.194
2.054	0.158	0.461	−0.18	0.511	0.154
2.316	0.133	0.504	−0.21	0.250	0.138
2.611	0.092	0.596	−0.24	0.038	0.218[a]
2.945	0.312	0.291	−0.27	−1.720	−0.172[a]

[a]Series questionable; see text.

give the same line in terms of the parameters j_0 and j_2. Column 5 gives the value of the exponent Θ_{R_x} as defined in Eq. (5). It was also obtained from the d log Padé analysis of (A1). Finally, in column 6, the surface tension along the roughening line Σ_R is given. Here Σ_R is

$$\Sigma_R = 2j_{0R} + 4j_{2R} - \sum_{n=2}^{7} a_n(x_R) y_R^n \ , \tag{6}$$

where $a_n(x_R)$ is obtained from the coefficient of y^n in (A2) evaluated at $x = x_R$. As our first observation, note from Table I that Σ_R is positive along the roughening line. In connection with our earlier discussion, this establishes the consistency of our low-temperature expansions.

Focusing specifically on Θ_{R_x} in Table I, both the magnitude and variation reflect shortcomings of the low-order series and the d log Padé approximant method used to study the series. The roughening exponent is known exactly for the body-centered solid-on-solid model to be $\Theta_{R_{\text{exact}}} = \frac{1}{2}$ [8], and is the expected result in our case along almost the entire roughening line except near the multicritical point. Near this point the theory is generally not well understood and so neither is the behavior of Θ_{R_x}. Excluding this region, the variation of the exponent can be understood in more precise terms by consideration of the crossover effects from the column modulated phases. For this note first that in the Ising limit the microscopic surface tension dominates, thus leading to the formation of the rough phase, which in particular implies a long correlation length. Next recall that in the column modulated phases the bending energy dominates the microscopic surface tension. Due to these opposing effects, as the magnitude of J_2 increases, the bending energy begins to compete with the microscopic surface tension, signifying the crossover effect referred to above. This in turn leads to shorter-ranged correlations or equivalently a decrease in Θ_{R_x}. Furthermore, the effects are much more pronounced in this system due to the presence of the Lifshitz point (L in Fig. 1), where the paramagnetic, ferromagnetic, and column modulated phases meet. One should expect that with a higher-order low-temperature expansion there would be less crossover behavior and so Θ_{R_x} should be more constant along the roughening line. Furthermore, this along with more sophisticated methods for series analysis, should give an exponent that is closer to its expected value of $\frac{1}{2}$.

Returning to Table I, observe that the last two rows of data show irregular behavior for which we can offer two mutually contributing causes. First, these points are close to phase boundaries which border other bulk phases and our series is expanded solely with reference to the bulk ferromagnetic phase. As such, crossover effects from other phases are influencing the validity of the expansion. In this context we also mention that the Lifshitz point, L in Fig. 1, may be having the greatest influence of all. The second reason for the unusual data is that the next-nearest-neighbor interaction is quite large here so that the auxiliary parameter x is large. As such, even though y is still small, its coefficient, which is a function of x, is now large. For example, in the second to last row the ratio,

$$r_{ij}(x,y) \equiv \frac{a_i(x) y^i}{a_j(x) y^j} \ ,$$

of the $i=7$ to the $j=6$ term for the series to Σ, Eq. (A2), is

$$r_{76}(x=2.611, y=0.092) = -0.45 \ ,$$

whereas for the last row,

$$r_{76}(x=2.945, y=0.312) = -1.99 \ .$$

This indicates that the smallness of successive terms is becoming questionable and that the series is at the limits of its validity.

In Fig. 1, line r is a sketch of the roughening line that was given in Table I. Its starting point at the zero of the abscissa is the Ising limit. As the next-nearest-neighbor coupling increases, the line slowly slopes downward. In terms of physical temperature, line r reads to say T_{R_x} decreases as the magnitude of the next-nearest-neighbor antiferromagnetic coupling increases but that the effect is gradual. Both these features can be qualitatively understood. The decrease in T_{R_x} for increasing next-nearest-neighbor antiferromagnetic coupling can be understood by consideration of the low-temperature expansion. One can easily see that the spins in the first two layers on either side of the interface are energetically unaffected by the second-neighbor coupling. In the third and further layers the antiferromagnetic coupling energetically favors spin flips thus weighing the balance towards a decrease in T_{R_x}. Naturally, such an argument applies to the bulk transition also, but since the roughening transition temperature is so much lower than the bulk critical temperature the argument is more sound. As for the slowness of the decrease in T_{R_x}, this is accounted for by the small connectivity of two with the second neighbors. In contrast, for the Widom model which has twelve diagonal and six second-neighbor couplings, the influence of these higher neighbor interactions on T_R is much greater [2].

III. CONCLUSION

To summarize, this paper has presented the low-temperature series for the second moment of $d\rho/dz$ and the surface tension Σ for an interface between two bulk ferromagnetic phases in the ANNNI model. We have obtained the roughening line and shown consistency of our results through establishing positive surface tension at T_{R_x}. The low-temperature series that we have presented are of general use for studies in real material. There are also several directions of further numerical investigation within the context of the roughening transition studied here. For one thing, our d log Padé analysis should mainly be trusted to give only a yes or no determination of the roughening singularity. To obtain better numerical accuracy would require further analysis by more sophisticated means. This would not merely be a numerical exercise but has importance for the calculation of the surface critical amplitude and exponent [3,6], where the precision in T_{R_x} is of the upmost importance. Another avenue of exploration relates to the study of L. What is needed here is an appropriate approximant that extends the validity of our series into the region near L much as the d log approximant did near the roughening transition.

Before concluding let us reflect on a few related thoughts. Ever since the work of Weeks, Gilmer, and Leamy [1], the presence of the roughening transition at the interface between bulk phases and its accessibility by low-temperature methods has been well accepted. Our work here and in Ref. [2,3] verify their findings and its interpretation as related to two-dimensional critical behavior. In terms of the latter point, our work serves as a check that higher neighbor interactions do not eliminate the singularity structure so found, though they do alter the value of the roughening critical exponent Θ_{R_x}. This is congruous to beliefs, although rigorously unproven but nevertheless well tested, about universality in critical phenomenon.

Placed with this confidence, let us extend our thoughts one further to the examination of similar two-dimensional singular behavior in bulk layered phases. As the first impediment, the low-temperature expansions called for there are nontrivial when it is noted that our own calculation involving the ferromagnetic phase required several long computer programs and elaborate hand counting. On the other hand, the layered case is more intriguing and most likely has concealed a much richer singularity structure. The mere fact that this may be accessible by the low-temperature approach prompts attention since it gives us a rigorous handle on the partition function. Due to the recent surge to model surface critical phenomenon, guidance from rigorous results such as these already justifies the benefit of the low-temperature expansion approach.

ACKNOWLEDGMENTS

A.B. thanks Professor Michael Fisher for helpful comments. We also thank Professor Kenneth A. Dawson for helpful discussions and for use of his computer facilities. Funding was provided to A.B. by the Department of Education and B.K. from the Regents of the University of California. Partial funding was also provided by the Sloan Foundation.

APPENDIX

The low-temperature series for the second moment of the density gradient as defined in Eq. (4) is

$$\langle z^2\rangle=[2]y^2+[14-8x]y^3+[40]y^4+[190+12x-58x^2]y^5+[812-92x+106x^2]y^6+[3604+172x-50x^2-456x^3]y^7 \ . \tag{A1}$$

The low-temperature series for the surface tension Σ is

$$\frac{\Sigma}{kT}=2j_0+4j_2-\{[2]y^2+[6-4x]y^3+[10]y^4+[27+2x-13x^2]y^5 +(\tfrac{209}{3}-10x+21x^2)y^6+[196+24x-6x^2-64x^3]y^7\} \ . \tag{A2}$$

*Present address: Department of Physics, University of Arizona, Tucson, AZ 85721.

[1] J. Weeks, G. H. Gilmer, and H. J. Leamy, Phys. Rev. Lett. **31**, 549 (1973).
[2] B. Kahng, A. Berera, and K. A. Dawson, Phys. Rev. A **42**, 6093 (1990).
[3] A. Berera and B. Kahng, Phys. Rev. A **46**, 4528 (1992).
[4] W. Selke, Phys. Rep. **170**, 1213 (1988).
[5] B. Widom, J. Chem. Phys. **84**, 6943 (1986).
[6] L. J. Shaw and M. E. Fisher, Phys. Rev. A **39**, 2189 (1989).
[7] J. L. Martin, in *Phase Transition and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1972), Vol. 3; S. Redner, J. Stat. Phys. **29**, 309 (1982).
[8] P. J. Forrester, J. Phys. A **19**, L143 (1986); J. Suzuki, J. Phys. Soc. Jpn. **58**, 3111 (1989).