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Reevaluation of series expansions for roughening transitions

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Ninth-order low-temperature series expansions for the Ising interface and SOS (solid on solid) models were once thought to be a suitable method for determining the location and exponents of the roughening transition. However, the temperature and exponent estimates thus derived were found to fail to obey exact, rigorous inequalities derived by Swendsen from Lapunov inequalities, and this led to obvious doubts as to the reliability of the estimates from such short series. In this Rapid Communication I show that a careful reanalysis of the series gives temperature and central-exponent estimates that obey the Swendsen-Lapunov inequalities, and are in excellent agreement with Monte Carlo and renormalization-group estimates. This reanalysis gives the first reliable estimate of the difference in the Ising interface and SOS roughening temperatures, within the same approximation. I find $Y_R(\text{Ising})=0.199\pm0.010$ $[T_R(\text{Ising})=2.475\pm0.075]$, and $Y_R(\text{SOS})=0.207\pm0.009$ $[T_r(\text{SOS})=2.54\pm0.07]$.

More than ten years ago low-temperature series expansions appeared to show great promise as an analytic tool for probing the nature and location of roughening transitions in Ising interfaces[1] and SOS[2] (solid on solid) models. The analysis of these series was based on the assumption that the interface width (W) diverges as

$$W \sim (T-T_R)^{-\theta} \tag{1}$$

at the roughening transition at temperature T_R. The series for the three-dimensional (3D) Ising-model interface[1] were generated for the first two moments $\langle z^2\rangle$ and $\langle z^4\rangle$ of the density gradient, and for the inverse of the gradient of the density at the center of the interface, M. M is found via the relation $M=1/[1-2\rho(z-\frac{1}{2})]$ with the $T=0$ interface located at $z=0$ and $\rho(z)$ the normalized layer density. The θ exponents for these three width measures are denoted by θ_2, θ_4, and θ_M, respectively. For the SOS model,[2] $\langle z^4\rangle$ series are not publically available.

It should be noted that in the years intervening between the presentation and subsequent discrediting[3] of the roughening series, and the present time, considerable developments have occurred in our understanding of the roughening transition. These are summarized in the reviews[4] of van Beijeren and Nolden and Balibar and Castaing. It is pertinent to our discussion to note that Chiu and Weeks[5] have mapped the double Gaussian roughening model onto a two-dimensional Coulomb gas, thus providing an upper bound for T_R for the SOS model. A lower bound for T_R for the SOS model was found by van Beijeren[6] to be the critical temperature of the two-dimensional Ising model. A summary of published T_R and θ estimates from the series, as well as other calculations, is given in Table I.

Swendsen[3] has shown that Lampunov inequalities can be derived to relate the kth and $k+1$st moments of the density gradient. These imply (if T_k is the temperature at which $\langle |z|^k\rangle$ diverges)

$$T_k \ge T_{k+1} , \tag{2a}$$

and

$$T_M \ge T_1 . \tag{2b}$$

If $T_i=T_M$ for all i then

$$\theta_k/k \le \theta_{k+1}/k+1 , \tag{2c}$$

and

$$\theta_1 \ge \theta_M . \tag{2d}$$

These inequalities can also be derived quite trivially if scaling is assumed, and Swendson's results have quite excluded the possibility of scaling violation. Observation of the results summarized in Table I shows that 2(a) and 2(b) are not satisfied by the results of Refs. 1 and 2. I quote Swendsen in saying that if the temperatures are set to a single biased estimate convergence is poor and 2(c) and 2(d) are also violated. (It is immaterial which pair of θ estimates from within the range of Ref. 1 are chosen, as all violate the inequalities.) These contradictions of the exact inequalities were interpreted as implying that the series were too short for reliability. This is disappointing, especially since Monte Carlo results[7] for the SOS model found T_R in reasonable agreement with the series estimate, and there is good agreement with the Monte Carlo results well below T_R. A glance at Table I shows that in addition to the inequality violations there is no clear consensus whether there is a single T_R for M, $\langle z^2\rangle$, and $\langle z^4\rangle$ or whether $T_R(\text{Ising})$ is larger or smaller than $T_R(\text{SOS})$. The series results are inconsistent; the SOS and Ising Monte Carlo T_R have been evaluated by somewhat different approaches, and the renormalization group (RG) does not evaluate T_R. It would be expected that $T_R(\text{Ising})$ is less than $T_R(\text{SOS})$ since there are additional excitations in the Ising systems, but the difference may be extremely small.

In this Rapid Communication I show that a reanalysis of the extant series gives central exponent estimates that satisfy the Swendsen-Lapunov inequalities. In addition,

TABLE I. Estimates for T_R, Y_R, and θ from different measures of the interface width, and from $G(r)$, the height-height correlation at distance r.

Measure	$k_B T_R/J$	$Y_R = \exp(-4J/k_B T_R)$	θ	Analysis	Ref.
		Ising interface			
M	2.46	0.1967	0.78	d log Padé	Weeks *et al.* (Ref. 1)
$\langle z^2 \rangle$	2.60	0.2147	1.00	d log Padé $\langle z^2 \rangle / Y^2$	Weeks *et al.* (Ref. 1)
$\langle z^4 \rangle$	2.64	0.219	1.43	d log Padé $\langle z^4 \rangle / Y^2$	Weeks *et al.* (Ref. 1)
		SOS interface			
M	2.4904	0.2006	0.972	Ratio	Leamy *et al.* (Ref. 2)
$\langle z^2 \rangle$	2.5568	0.209	0.968	Ratio	Leamy *et al.* (Ref. 2)
		RG estimates			
M	...	...	$\frac{1}{4}$		Ohta and Kawasaki (Ref. 9)
$\langle z^2 \rangle$	...	...	$\frac{1}{2}$		Ohta and Kawasaki (Ref. 9)
$\langle z^4 \rangle$	...	...	1.0		Ohta and Kawasaki (Ref. 9)
		Monte Carlo			
ASOS $G(r)$	2.48	0.199	...		Shugard *et al.* (Ref. 7)
ASOS W	2.28	0.17	...		Swendsen (Ref. 3)
Ising W	2.42 ± 0.12	0.19 ± 0.02	...		Burkner and Stauffer (Ref. 14)
		Exact			
2D Ising (lower bound)	2.26	0.17	...		Van Beijeren (Ref. 6)
DG (upper bound)	2.90	0.25	...		Chui and Weeks (Ref. 5)

single and distinct central T_R estimates are made for the Ising and SOS models, although the error bars are such that equality cannot be completely excluded. Faith in the series is therefore restored and two useful T_R estimates are made.

One possible explanation for the problems with the series is that it is not the series themselves which are suspect, but rather their analysis. After all, it has been shown that roughening transitions have essential singularities;[4] in this event Eq. (1) would be incorrect, and any analysis based on it would therefore be unreliable. Methods have been developed[8] to study the asymptotic behavior of series with essential singularities. I was somewhat surprised to find that attempts to analyze the various series by looking at the double logarithmic derivative[8] clearly showed that these series have power-law singularities in agreement with Eq. (1). In fact, Ohta and Kawasaki[9] have given RG arguments to show that the interface widths measured by the moments of the density profile and by the inverse of the gradient of the profile at the center of the interface all have critical behavior of the form of Eq. (1) and do not exhibit essential singularities. They suggest that $\theta_M = \frac{1}{4}$, $\theta_2 = \frac{1}{2}$, and $\theta_3 = 1.0$; these values are consistent with the Lapunov inequality as an equality and are each exactly $\frac{1}{2}$ of the corresponding mean-field exponents. Thus it is somewhat perplexing that the series failed to give exponent estimates anywhere near these values; the series estimates for θ_M of 0.78 and 0.972 being at least 3 times as large as the RG result. This is a far larger discrepancy than that between series and RG results in, for example, 2D percolation.

The problems in the early Ising and percolation-series analyses were caused by neglect of allowance for irrelevant operators in the series analyses.[10] Allowance for these operators means replacing Eq. (1) with the assumption that W diverges as

$$W \sim (T - T_R)^{-\theta}[1 + a(T - T_R)^{\Delta_1}] \ . \tag{3}$$

We have no idea in advance what value Δ_1 will take for interface widths but may conjecture[11] that it will take the same value for the different moments (as appears to occur in percolation series), although not necessarily for M.

We shall carry out the analysis of the series based on Eq. (3) by the following two different methods: $M1$,[12] essentially designed to estimate Δ_1, and $M2$,[10] designed to remove the influence of the correction on the estimation of θ. In both cases we will obtain graphs of different Padé approximants to θ as a function of input Δ for a chosen value of T_R. These different Padé approximants will converge near the correct (θ, Δ) estimate, and the values of T_R and Δ that give the tightest convergence are the correct T_R and Δ_1. The θ value for $\Delta = 1.0$ corresponds to the result from a temperature-biased d log Padé analysis.

Some thought must also be given to the form in which to cast the series for their analysis. The $\langle z^2 \rangle$ and $\langle z^4 \rangle$ series here are of the form

$$a(0) + a(1)Y + a(2)Y^2 + \cdots \ ,$$

where $Y = \exp(-4J/k_B T)$ is the low-temperature variable, and $a(0) = a(1) = 0$. As far as I can determine, the d log Padé analysis of Ref. 1, Table II, has been carried out on the series divided by the square of the expansion variable Y, perhaps so that the first term studied is a constant. This could, and in my opinion has, led to severe systematic errors in the determination of the exponents.

Since the algorithms of $M1$ and $M2$ also require that the first term of the series be a constant, I have looked at their second derivatives, and at the series $\pm$ some arbitrary constant C as well as the series/Y^2.

From Table I we can see that there is quite a large range of T_R estimates in the literature. I have studied the various θ's as functions of Δ throughout this range, and have looked at Δ_1 estimates between 0.2 and 6.0 using both $M1$ and $M2$. If the series are long enough we should find optimal convergence for a tight range of θ, Δ_1, and Y_R for each series, and we should obtain the same numbers from both methods. For the nine-term series the convergence is not extremely tight, especially for Δ_1, but nevertheless central values and error ranges can be determined for each of these three quantities. It was a very pleasant surprise to observe that the central Y_R values for the three Ising series are very close, and although there appear to be two Δ_1 convergence regions for the M series and only one for the others, the central θ values deduced from the common Δ_1 region are extremely close to the RG values. I obtain $Y_R=0.199\pm0.010$ ($T_R=2.473\pm0.075$) and Δ_1 estimates to be discussed below. The $\langle z^2\rangle$ and M SOS series give $Y_R=0.207\pm0.009$ ($T_R=2.54\pm0.07$).

Selected graphs of θ as a function of Δ for certain Y_R choices are given in Figs. 1 and 2. In Fig. 1(a) a graph of θ_4 as a function of Δ for $Y_R=0.2$ using $M2$ is given, and in Fig. 1(b) a graph using $M1$ is presented. The $\langle z^4\rangle/Y^2$ series have been used in both these calculations. In Fig. 1(c) curves for $\langle z^4\rangle''$ with $M2$ are given. We observe that all these converge for $\theta_4=1.0\pm0.2$ and $\Delta_1=2.0\pm0.4$, as indicated by the boxes. This θ_4 is in pleasing agreement with the RG result. The usual Padé analysis would give $\theta_4\simeq0.9$ at these Y_R choices. (This is much lower than the value given in Ref. 1; the reason that the θ_4 of Ref. 1 is so much higher is that it corresponds to optimal convergence of Y_R and θ_4 for $\Delta=1$, but still better convergence can be achieved with variation of Δ_1.) The results of $M1$ with the $\langle z^4\rangle''$ series are consistent with the above and are less well converged. Figure 2 is devoted to the analysis of the $\langle z^2\rangle''$ series. In Fig. 2(a) we present the SOS analysis at $Y_R=0.206$ and in Fig. 2(b) the $\langle z^2\rangle''$ Ising analysis at $Y_R=0.199$; both figures are from $M2$, but the $M1$ results are quite consistent with these. The different $\langle z^2\rangle''$ plots for the SOS model in the range $Y_R=0.207\pm0.009$ give $\theta_2=0.50\pm0.15$, and for the Ising interface the range $Y_R=0.199\pm0.010$ gives $\theta_2=0.50\pm0.20$. The $\langle z^2\rangle/Y^2$ series gave poorer convergence to θ_2 values $\simeq0.7$ for both models. Graphs for the M series are not presented for space reasons. For the Ising model with $M2$ at $Y_R=0.190$ there is good convergence below $\Delta_1=2.0$, but at $Y_R=0.199$, $\Delta_1\simeq2.0$ corresponds to $\theta_M\simeq0.25$. For the SOS model at $Y_R=0.207$ $\Delta_1<1.0$ and $\theta_M=0.25\pm0.05$. For both models $M1$ suggests $\Delta_1\sim1.0$ implying that although there is no reason to suspect different irrelevant operators in the M and $\langle z^2\rangle$ and $\langle z^4\rangle$ series, the amplitudes may be very different. If the lower Δ_1 value is the correct one for the Ising M series then the conclusion that there is a single Y_R estimate for the three series has to be questioned. For the SOS series, however, there is no such problem; both the $\langle z^2\rangle$ and the M series give the same Y_R, and thus this does not seem very likely. We have given the

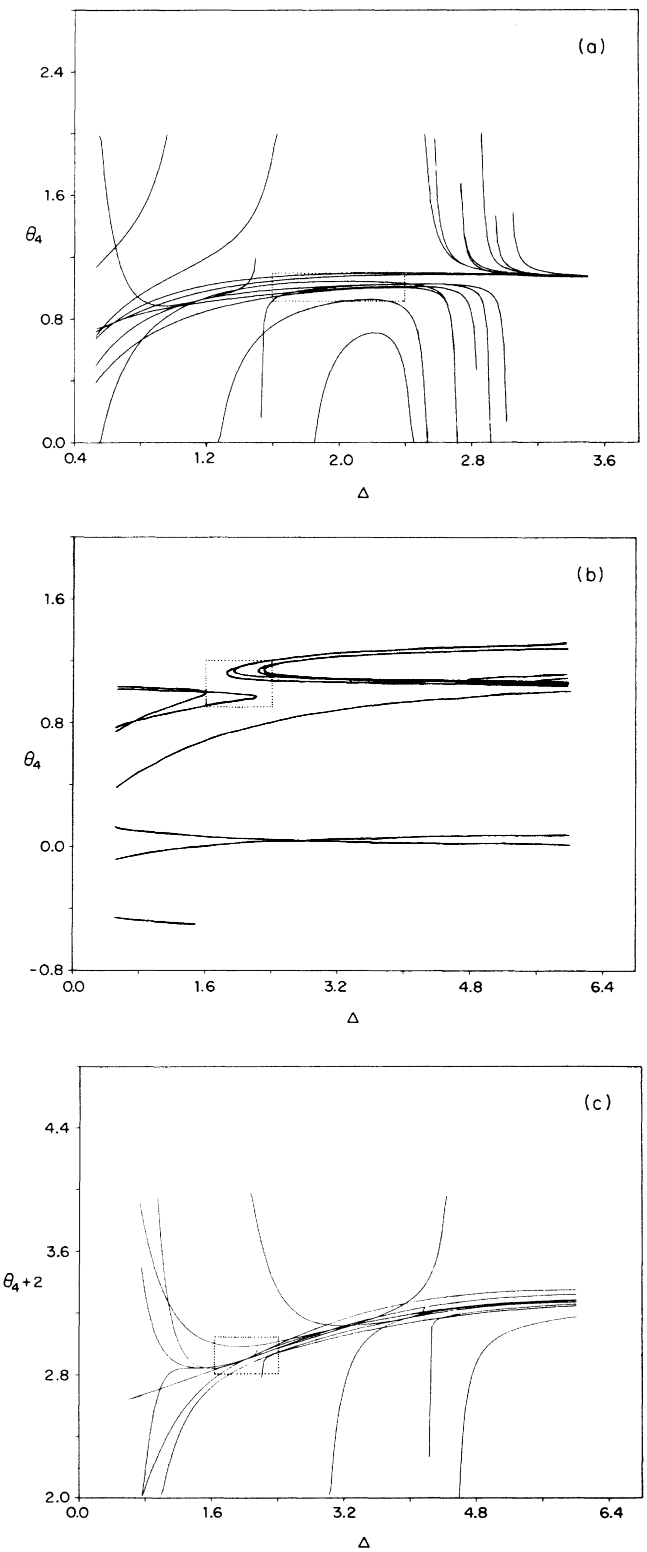

FIG. 1. Graphs of θ_4 as a function of Δ for (a) $\langle z^4\rangle/Y^2$(Ising) at $Y_R=0.200$ with $M2$, (b) $\langle z^4\rangle/Y^2$(Ising) at $Y_R=0.200$ with $M1$, and (c) $\langle z^4\rangle''$(Ising) at $Y_R=0.201$ with $M2$. Optimal (θ_4,Δ_1) choices for this Y_R are indicated by boxes.

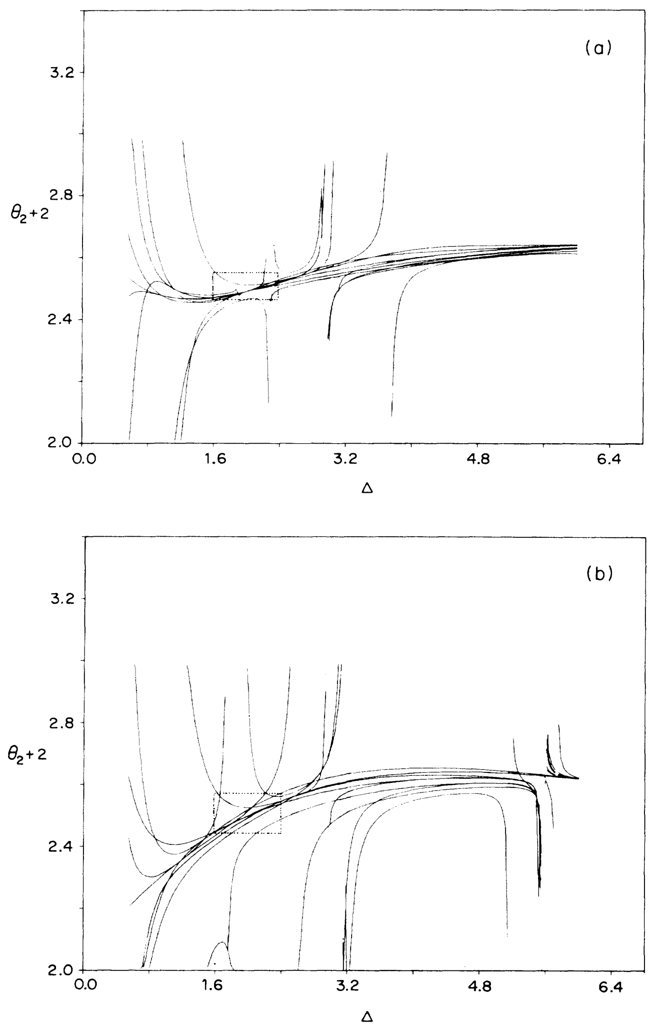

FIG. 2. Graphs of θ_2 as a function of Δ for (a) $\langle z^2\rangle''$(SOS) at $Y_R=0.206$ with $M2$, (b) $\langle z^2\rangle''$(Ising) at $Y_R=0.199$ with $M2$. Optimal (θ_2,Δ_1) choices for these Y_R are indicated by boxes.

overall estimates $\Delta_1=1.0\pm0.04$, $\theta=0.25\pm0.15$ for the M series.

I now consider the implications of these analyses. First, I have been able to find a single pair of T_R values for the Ising and SOS series at which the central θ values[13] are consistent with the Swendsen-Lapunov inequalities. Furthermore, these θ values include the RG results of Ohta and Kawasaki[9] at the center of their ranges, strongly suggesting that although the RG numbers may not be rigorous, they are probably exact. In addition, I have found T_R(Ising) and T_R(SOS) to be close but not identical. The SOS value is slightly higher than the Ising one, as expected. I note that the difference between the central $Y_R(T_R)$ estimates is 0.008 (0.065), which is smaller than the error bounds on either $Y_R(T_R)$. These error bounds are based on averaging the temperatures obtained from all the series by both analysis methods and thus are larger than the actual uncertainty in each measurement. If we compare either the $\langle z^2\rangle''$ or M series analyses for the SOS series with the corresponding Ising series, then it is clear that the T_R estimates are distinct for the two models. I note that of the previous T_R estimates, those of Refs. 2, 7, and 14 and the M series of reference are consistent with these new results, but the $\langle z^2\rangle$ and $\langle z^4\rangle$ estimates of Ref. 1 are above my range.

The SOS series are better behaved than the Ising ones, but I have demonstrated that from both series clear results, consistent with available exact Monte Carlo and RG results, can be obtained.

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