

# Tests for Monte Carlo Renormalization Studies on Ising Models

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In this expanded version of an earlier letter, we consider many computational details that were omitted for want of space. For  $d=2$  Ising spins with up to 13 different short-range interactions, we construct the critical surface in the vicinity of (Onsager's) nearest-neighbor (nn) critical point by using the body of the available information on the solvable nn case. We then see if the Monte Carlo renormalization group flows generated from this point do indeed lie on this surface and quantify the errors if they do not.

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**KEY WORDS:** Ising model; critical surface; Monte Carlo renormalization group; transfer matrix; correlation functions.

## 1. INTRODUCTION

The renormalization group (RG) provides us with a very satisfactory framework for describing critical phenomena.<sup>(1-4)</sup> A central idea in this approach is that given a hamiltonian  $H^0$  that describes interactions between degrees of freedom on a lattice, one can trade it for another hamiltonian  $H^1$ , that describes interactions between "block" degrees of freedom on a lattice with a spacing  $L$  times as large.  $H^0$  and  $H^1$  are equivalent for physics at distances beyond  $L$ . One can then trade  $H^1$  for  $H^2$  and so on. This leads to the notion of a flow under renormalization, in an infinite-dimensional space of parameters  $K=(K_1, K_2, \dots)$  where each coupling  $K_i$  describes a possible interaction. For example, for a system of Ising spins,  $K_1$  could be the nearest-neighbor (nn) coupling and so on. One next conceives of a critical surface (CS) in  $K$  space containing all critical Hamiltonians. If one starts with any point on this surface, the flow will be restricted to this surface since the dimensionless correlation length is  $\infty$  to begin with and  $\infty/L$  after blocking. More specifically there is a fixed point

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$H^*$  on this surface towards which all critical Hamiltonians will flow. Since all of them can be traded in for  $H^*$  for long distance physics, the difference  $H^0 - H^*$  is termed irrelevant. In contrast if  $H^0$  has a small component outside the CS this "relevant" parameter would get amplified with each iteration by a factor  $L^{1/\nu}$  where  $\nu$  is the correlation length exponent. Thus  $H^n$ , as  $n$  increases, will first track the CS, approach  $H^*$  and then veer away. Universality can be understood in terms of the vanishing under renormalization of irrelevant coordinates (measured from  $H^*$ ) and divergences (as  $H^0$  approaches the CS) can be understood in terms of the divergent amount of "time" the image point spends near  $H^*$  before veering away. (It should be noted that while the CS and critical indices are universal,  $H^*$  depends on the blocking procedure adopted.) It will be gratifying to test this geometrical picture of flows whenever possible. To do so analytically is impossible in all but a few cases. The problem is that even a simple nn  $H^0$  becomes, upon renormalization, a highly complicated interaction. Only the pure Gaussian interaction is free of this problem and remains Gaussian under a momentum space reduction of degrees of freedom. Another situation where things are somewhat under control is the  $\varepsilon$  expansion, where, to a given order in  $\varepsilon$ , the flow equations and fixed point can be restricted to a subspace of  $K$ . In the general case, say the  $d=2$  Ising system, one must resort to a brutal truncation to keep things tractable.

Numerical Monte Carlo methods are relatively free from these problems. Recently some very creative methods have been devised for extracting the block spin hamiltonian.<sup>(5,6)</sup> As many as 14 most significant interactions have been extracted in  $d=2$  and 17 in  $d=3$  in high-precision studies. It is also possible to iterate as many as three times. Even if the flow is deduced numerically, we still need to know the CS before we can one ask if these flows and projected fixed points indeed are restricted to the CS if the starting  $H^0$  is critical, and if any small component of  $H^0$  outside the CS gets amplified as per the scaling laws.

This is precisely what we did for  $d=2$  Ising spins in Ref. 7. We provide many details in this expanded version. Using the vast body of available information on the solvable nn problem we construct the equation for the CS in the vicinity of the nn transition at  $K=(0.440687,0,0,0\dots)$ . More precisely, we derive the equation for the tangent plane at this point in Section 2 and curvature corrections in Section 3. In Section 4 we inquire if the block Hamiltonian generated from a critical nn system by the above-mentioned MCRG studies do indeed lie on this surface and if not, we quantify the errors. Likewise, if some truncated block Hamiltonian is simulated, we can quantify the relevant variable and ask if it grows according to scaling laws upon iteration.

A by-product of our analysis is the notion of a metric in  $K$  space. The

metric factor  $g_i$  converts every coupling  $k_i$  to a “physical” value  $k'_i = g_i k_i$ , where  $k'_i$  is a truer measure of its importance, i.e., measures its contribution to the singular part of the free energy. (Here all  $k_i$  are measured from the nn critical point.) Thus a coupling can be said to be small in a physical sense if the metricized value  $g_i k_i$  is small. Likewise if criticality is lost, say by the reduction of some  $k'_i$  by a small amount, it can be restored by increasing any other  $k'_j$  by the same amount. This will be discussed on Section 2.

There is another question we partly answer: even though (metricized) individual terms corresponding to more distant and complicated interactions can be small, could they be safely neglected or could they, as a group, produce big effects due their large numbers? The answer seems negative at least in the limited context that we study in Section 4.

The final point we address (in Section 5) is the following. In searching for a fixed point, one begins with a critical nn system and starts iterating. There are two routes to follow here. In the first one always simulates the nn system, and having obtained the configurations forms the block spins and extracts the block Hamiltonian. To block again one does not simulate with the block Hamiltonian, one simply does one more blocking. The advantage of this method is that one never leaves the critical surface (except for size effects). One does not even have to ask what the block Hamiltonian is at each stage. Stated differently, if only the first ten interactions can be unearthed without sizable errors, the neglect of the others does not constitute a truncation error that grows, since every interaction that can fit into the given lattice is really there, it is just not extracted or reported. The drawback in this scheme is that with each blocking the lattice size diminishes. The second approach tries to beat this by simulating the block Hamiltonian on the original lattice. Now the problem is with the inevitable truncation in the Hamiltonian being simulated and the magnification of this error with further iteration.

For  $d=2$  our detailed knowledge of the critical surface allows us to propose a truncation scheme that will put one back on the critical surface after every iteration and truncation. (There is, however, a cruder scheme, which gives nearly the same results but is not predicated on such detailed knowledge. One could explore the possibility of applying it in  $d=3$ .)

## 2. THE TANGENT PLANE AND METRIC

We illustrate the procedure for obtaining the tangent plane in the  $K_1-K_2$  (nn- $\text{nnn}$ ) subspace. The partition function is

$$e^{Nf} = Z = \sum_s \exp(K_1 \sum_s s s_{nn} + K_2 \sum_s s s_{nnn}) \quad (2.1)$$

If  $K_2 = 0$ , the problem is solvable. There is a phase transition at  $K_{1c} = 0.440687$  with a logarithmic singularity in the specific heat. This point belongs to the CS in the  $K_1$ - $K_2$  plane. Our aim here is to determine the tangent to this CS. First observe that

$$f' = df/dK_1 \quad (2.2)$$

(where  $f$  is the free energy per site) will have a logarithmic singularity in its  $K_1$  or  $K_2$  derivative as we approach  $K_{1c}$  along the  $K_1$  axis. This is because in either case we are differentiating  $f'$  with respect to the relevant variable. By the same token the directional derivative along the tangent to the CS will be free of singularities since we are differentiating with respect to the irrelevant variable. If we consider a point on the  $K_1$  axis a distance  $\delta$  from  $K_{1c}$  we will find that while both  $K_1$  and  $K_2$  derivatives will diverge as  $\delta \rightarrow 0$ , a certain linear combination will be divergence free. This combination specifies the tangential direction. To find  $\partial f'/\partial k_i$  ( $i = 1, 2$ ) we use

$$\partial f'/\partial K_i = \partial^2 f/\partial K_i \partial K_1 = \partial^2 f/\partial K_1 \partial K_i = \partial(2\langle H_i \rangle)/\partial K_i \quad (2.3)$$

where  $H_1 = ss_{nn}$  and  $H_2 = ss_{nnn}$  are the interactions that multiply  $K_1$  and  $K_2$  in the energy formula, Eq. (2.1). (The factor of 2 arises because at each of the  $N$  sites there are two terms of the form  $H_i$  associated with two independent directions.) We know that<sup>(8)</sup>

$$\begin{aligned} 2\langle ss_{nn} \rangle &= \sqrt{2} - 8/\pi(\delta \ln \delta - 3 \delta^2 \ln \delta/\sqrt{2}) + O(\delta^3) \\ 2\langle ss_{nnn} \rangle &= 4/\pi(1 - 2\sqrt{2} \delta \ln \delta + 6 \delta^2 \ln \delta) + O(\delta^3) \end{aligned} \quad (2.4)$$

It follows that along the tangent plane

$$A \equiv k_1 + \sqrt{2} k_2 = 0 \quad (2.5)$$

where  $k_1$  and  $k_2$  are measured from  $(K_{1c}, 0)$ ,  $f'$  has a finite derivative.

The extension of Eq. (2.5) to more couplings is direct: (i) one computes  $m\langle H_i \rangle$ , where  $m$  is the multiplicity and  $H_i$  the corresponding interaction; (ii) one takes the  $k_1$  derivative at the point  $K_{1c} + \delta$  and picks out the coefficient of the  $\ln \delta$  term, dropping an overall factor of  $-8/\pi$ . For any multispin interaction,  $m$  is chosen so that every interacting doublet, quartet, sextet, etc. is represented exactly once. In contrast to  $\langle H_1 \rangle$  and  $\langle H_2 \rangle$  which are readily available, the others had to be computed. We relied on Itzykson's paper<sup>(9)</sup> on the Ising model to compute  $\langle H_i \rangle$ . An example is given in Appendix A. Table I contains the values  $g_1$  through  $g_{13}$ , where  $g_i$  are the coefficients in the equation for the tangent plane:

$$A \equiv \sum g_i k_i = 0 \quad (2.6)$$

Table I. Metric Coefficients for 13 Coupling Ordered According to Range.<sup>a</sup>

0 1 2 3 4 5 6 7 8	$g_i$	
$k_1 = k_{01}$	1	1.0000
$k_2 = k_{04}$	$\sqrt{2}$	1.4142
$k_3 = k_{0134}$	$2\sqrt{2}(1-2/\pi)^* 1/2$	0.5139
$k_4 = k_{02}$	$4\sqrt{2}/\pi$	1.8006
$k_5 = k_{1345}$	$(8/\pi - 1)^* 2$	3.0930
$k_6 = k_{1357}$	$4\sqrt{2}(4/\pi - 1)^* 1/2$	0.7728
$k_7 = k_{05}$	$2^* 2$	4.0000
$k_8 = k_{0145}$	$\sqrt{2}^* 2$	2.8289
$k_9 = k_{0457}$	$4\sqrt{2}/\pi^* 2$	3.6000
$k_{10} = k_{0157}$	$(8/\pi - 1)^* 4$	6.1859
$k_{11} = k_{0123}$	$\sqrt{2}^* 4$	5.6569
$k_{12} = k_{08}$	$16\sqrt{2}/3\pi$	2.4008
$k_{13} = k_{0148}$	$16/3\pi^* 4$	6.7906

<sup>a</sup> Multiplicity factors (*relative* to the first term) are shown explicitly following the \*. For example there are eight per site of the form 0148.

We would like to view  $g_i$  as the metric (near the nn transition) that converts any  $k_i$  to a more physical  $k'_i = g_i k_i$  that is a truer measure of its significance in controlling the singular part of the free energy. For example in the  $K_1$ - $K_2$  plane we see that if criticality is lost by a change  $\delta k_1$  in  $k_1$ ; it can be restored by a compensating change  $\delta k_2 = -\delta k_1/\sqrt{2}$ . Thus  $k_2$  is  $\sqrt{2}$  times more effective than  $k_1$ , and  $k'_2 = \sqrt{2} k_2$  is a better measure of this term.

### 3. QUADRATIC CORRECTIONS

The tangent plane that we determined in Section 2 will fail to be a good approximation to the CS as we move further out from the point of tangency. We now derive the first corrections due to the curvature of the CS. These will turn out to be rather small (for the excursions in MCRG studies). Let us begin in the 1-2 plane again. In the tangent approximation, the CS is given by

$$k_2 = -(1/\sqrt{1}) k_1 + O(k_1^2) \quad (3.1)$$

We will now derive the coefficient of the  $k_1^2$  term. Consider a point  $(k_{1c} + \delta, 0)$ . Let some curve  $[k_1(t), k_2(t)]$  pass through this point, where  $t$  is a parameter that vanishes at this point. Suppose we compute  $df'/dt$ . We will find that it has a logarithmic singularity as  $\delta$  vanishes:

$$df'/dt = k_{1,t} \partial f' / \partial k_1 + k_{2,t} \partial f' / \partial k_2 \quad (3.2a)$$

$$= -(8/\pi)[k_{1,t} \ln \delta + \sqrt{2} k_{2,t} \ln \delta] + O(\delta) \quad (3.2b)$$

where  $k_{i,t} = dk_i/dt$ . However the  $\ln$  singularity vanishes if

$$k_{1,t} + \sqrt{2} k_{2,t} = 0 \quad (3.3)$$

i.e., if the curve has the same tangent as the CS. Let us now repeat this analysis for  $d^2f'/dt^2$ . We will find that singularities are present in general but can be eliminated on a curve of a particular curvature. The latter is, of course, the curvature of the CS that we are seeking. Here are the details. Differentiating Eq. (3.2a) with respect to  $t$  we get

$$\begin{aligned} d^2f'/dt^2 &= k_{1,tt} \partial f' / \partial k_1 + k_{2,tt} \partial f' / \partial k_2 + (k_{1,t})^2 \partial^2 f' / \partial k_1^2 \\ &\quad + (k_{2,t})^2 \partial^2 f' / \partial k_2^2 + k_{1,t} k_{2,t} \partial^2 f' / \partial k_1 \partial k_2 \\ &\quad + k_{2,t} k_{1,t} \partial^2 f' / \partial k_2 \partial k_1 \end{aligned} \quad (3.4)$$

As  $\delta \rightarrow 0$  one can expect  $\ln \delta$  and  $\delta^{-1}$  singularities. The latter will however cancel automatically given that  $k_{1,t} + \sqrt{2} k_{2,t} = 0$ . To see this, consider the sum of the third term and fifth terms, where we can expect a  $\delta^{-1}$  singularity.

$$(3) + (5) = k_{1,t} \partial / \partial k_1 [k_{1,t} \partial f' / \partial k_1 + k_{2,t} \partial f' / \partial k_2] \quad (3.5)$$

However the term in brackets is free of  $\ln \delta$  singularities since  $k_1$  and  $k_2$  are in the ratio  $1: -1/\sqrt{2}$ . Thus, differentiating with respect to  $k_1$  (i.e.,  $\delta$ ) will only produce a  $\ln$  term. A similar argument can be applied to the sum of the fourth and sixth terms. In short we must compute all the  $\ln \delta$  terms in right-hand side of Eq. (3.4) and set them to zero. The  $\ln \delta$  terms in  $\partial^2 f' / \partial k_1^2$  and  $\partial^2 f' / \partial k_1 \partial k_2$  can be read off Eq. (2.4), they are  $-3\sqrt{2}$  and  $-6$  (upon dropping the usual factor of  $-8/\pi$ ). The tedious computation of the singular part of  $\partial^2 f' / \partial k_2^2 = \partial^3 f / \partial k_1 \partial k_2^2$  is described in Appendix B. The resultant value is  $-4\sqrt{2}(1 + 2/\pi)$ . Let us now return to Eq. (3.4) with these results. Since  $t$  is any acceptable parameter let us trade  $t$  for the function  $k_1(t)$ , i.e., use  $k_1$  as the parameter on the curve.

We get, upon setting  $dk_2/dk_1 = -1/\sqrt{2}$ , the following coefficient for the  $\ln \delta$  term (on dropping the usual factor of  $-8/\pi$ )

$$k_2'' \sqrt{2} - 3 \sqrt{2} + (1/\sqrt{2})(2)(6) + (-1/\sqrt{2})^2(-4 \sqrt{2})(1 + 2/\pi)$$

This implies

$$k_2'' = (4/\pi - 1) \tag{3.6}$$

where primes denote differentiation with respect to  $k_1$ .

The equation for the CS therefore is

$$k_2 = -(1/\sqrt{2}) k_1 + 1/2(4/\pi - 1) k_1^2 + O(k_1^3) \tag{3.7}$$

which can be rewritten

$$\Delta = 2^{-1/2}(4/\pi - 1) k_1^2 = 0.19321 k_1^2 \tag{3.8}$$

in terms of  $\Delta \equiv \sqrt{2} k_2 + k_1$ . If we now define a metric distance  $d$  by

$$d^2 = \sum_i (g_i k_i)^2 \tag{3.9}$$

we can write Eq. (3.8) as

$$\Delta = (2^{-3/2})(4/\pi - 1) d^2 = 0.09660 d^2 \tag{3.10}$$

since on the surface  $d^2 = k_1^2 + (\sqrt{2} k_2)^2 = 2k_1^2 + O(k_1^3)$ .

Our motivation for rewriting Eq. (3.8) as Eq. (3.10) is the following: In most of the MCRG studies  $k$  is not confined to the 1–2 plane though it is almost entirely in it. In such a situation we can expect that an equation like (3.10) will hold, but with a coefficient  $\alpha(\theta)$  for the  $d^2$  term, where  $\theta$  measures the angle out of the 1–2 plane. Now if this angle is small (even after metricizing the lengths), we can assume that  $\alpha(\theta)$  is approximately equal to  $\alpha(0) = (4/\pi - 1)/2 \sqrt{2}$ . Now in most of the cases the length of  $k$  in the 1–2 plane is 95%–98% of the full length and we will set  $\alpha(\theta) = \alpha(0)$ . The numerical value of this term is confined to the range 0.002–0.003. This suggests that any corrections due to nonzero  $\theta$  or higher orders in  $d$  are very much smaller. (The numerical uncertainties in  $\Delta$  in today’s best data are around 0.001.) We are now ready to perform a comparison of Eq. (3.10) with the MCRG results.

#### 4. COMPARISON WITH NUMERICAL WORK

We begin with the well-known fixed point of Nauenberg and Nienhuis<sup>(10)</sup> which has components  $K_1 \equiv K_{01} = 0.307$ , i.e.,

$k_1 = 0.307 - 0.441 = -0.134$ ;  $k_2 = K_2 = k_{04} = 0.084$ ; and  $k_3 = K_3 = k_{0134} = -0.004$ . We get  $\Delta = -0.017$ . Since the vector is 99% in the 1-2 plane, we safely use Eq. (3.10) which predicts  $\Delta = 0.002$ . So the error in  $\Delta$  is 0.019. This translates to a 5% error in the following sense. (This was suggested to us by Professor Swendsen.) Suppose we take a point on the CS (so that  $\Delta = 0.002$ ) and rescale  $K$  by 1%. This changes  $\Delta$  by roughly 1% of  $K_{1c} = 0.440689$ , i.e., by 0.004. So an error of 0.019 is roughly a 5% effect. Next consider Callaway and Petronzio,<sup>(11)</sup> who found a novel way to extract the renormalized couplings. Their fixed point is at  $k_1 = -0.12 \mp 0.01$  and  $k_2 = 0.07 \mp 0.01$ . The error is again around 5%.

We now turn to the highly accurate results of Swendsen<sup>(5)</sup> and of Gupta and Corderey.<sup>(6)</sup> Swendsen starts on a  $32 \times 32$  lattice with a critical nn system. Having generated the configurations, he blocks the spins ( $2 \times 2$  blocking) and extracts the block Hamiltonian by a method devised by him. He reports seven couplings:  $k_1$  through  $k_7$  (except  $k_5$ ) and  $k_{12}$ . The  $\Delta$  for three of these sequential blockings is 0.004, 0.005 (This time  $k$  was 98% in the 1-2 plane). The expected values for  $\Delta$  are 0.002, 0.003, and 0.003, respectively. Thus the errors are of the order of 0.5%. They do not grow with each blocking since the Hamiltonian simulated is always a critical nn Hamiltonian. Of course the lattice size decreases to  $4 \times 4$  after the third blocking. However there is no visible growth in  $\Delta$  due to this finite size effect.

He also gives results of  $3 \times 3$  blockings: twice on a  $36 \times 36$  lattice and once on a  $12 \times 12$  lattice. Here however  $k$  has a sizable out of plane component and hence we cannot compute  $\Delta$  reliably. If we ignore this, the expected  $\Delta$ 's are 0.002, 0.003, and 0.002 compared to "measured" values of 0.001,  $-0.006$ , and 0.000. Notice that in the  $2 \times 2$  case the flow is slightly above the CS while in the  $3 \times 3$  case it seems to be below the CS.

Now for Gupta and Corderey who give us the results of three studies  $G(1)$ ,  $G(2)$ , and  $G(3)$ . In  $G(1)(G(2))$   $2 \times 2$  blocks are formed on a  $32 \times 32(64 \times 64)$  lattice starting with a critical nn system. Fourteen different block interactions are deduced by yet another method. The calculated  $\Delta$  is 0.0020 in all the three cases due 13 terms. The tiny effect due to the 14th will be discussed later. The measured values were 0.0087, 0.0061, and 0.0144. (The  $k$  vector was 95% in the 1-2 plane).

However these numbers do not give the complete picture; for that we must turn to Fig. 1, which shows how  $\Delta$  changes as we include more and more terms in the order of increasing range (defined as the largest separation between any two spins in interaction.) When many terms of a given range are encountered, couplings with fewer spins get precedence and further degeneracies are resolved by seeking that orderings of terms which favours oscillations in sign.



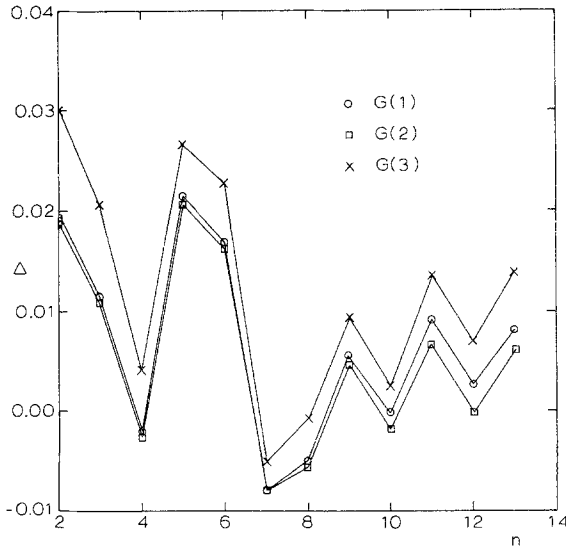


Fig. 1. Variation of  $\Delta$  as more and more interactions are included in the sum. In  $G(1)$  ( $G(2)$ )  $2 \times 2$  blocks are formed on a critical  $32 \times 32$  ( $64 \times 64$ ) lattice with  $nn$  interactions. In  $G(3)$   $2 \times 2$  blocks are formed keeping only 14 interactions extracted from  $G(2)$ .

The best way to summarize  $G(1)$  is to say that  $\Delta$  oscillates around a value of 0.005. The graph suggests that if more terms were included the oscillations would converge to 0.005. The error would be 0.75%. We can see that not only do individual contributions seem to decrease with range, but also that there are big cancellations within each range. (In  $\Delta$ , opposite couplings tend to cancel since the  $g_i$  are all positive due to Griffiths' inequalities).<sup>(12)</sup>

Consider now  $G(2)$ . Here the oscillations are about 0.003, i.e., the error is 0.25%. We attribute the improvement to the doubling in lattice size which alters the last half a dozen couplings.

As for  $G(3)$ , which is obtained by simulating the truncated Hamiltonian deduced in  $G(2)$ , the input error is 0.004. [The last point on the graph of  $G(2)$  and not the average, gives the input error.] By scaling theory, this will get amplified in a  $2 \times 2$  blocking to  $0.004 \times 2^{1/b} = 0.008$ . So we expect that  $G(3)$  will correspond to oscillations about  $\Delta = 0.010$  which seems to be the case. (Had we included the fourteenth coupling with its estimated contribution of 0.001, the expected  $\Delta$  would have been 0.012.)

The figure also suggests a way by which the authors could have improved matters in computing  $G(3)$  from  $G(2)$ . Suppose they had altered the last coupling such that  $\Delta$  came down to 0.002 (instead of being at 0.006). This would have converted a relevant error (arising from the neglect

of all smaller interactions) to an irrelevant error (in the last component, which they altered to get back on the CS). Of course, in this  $d=2$  case where the critical exponents are known, the only point in doing this would be to see how well numerical studies could perform given a way to get back on the CS after every iteration.

There is a more ad hoc but possibly more generalizable prescription. Suppose the feature we see in the figure, namely that as more and more terms are included  $\Delta$  will oscillate around the correct value (by correct we mean the best one can do given the finite lattice size) and that these oscillations are roughly symmetrical. Then a good rule of thumb one can follow even if  $g_i$  are unknown would be the following: assemble all the couplings according to range, choosing in case of a tie that order that promotes oscillations and simply reduce the last reliably measured term to half its value if an oscillatory pattern has set in. When applied to the thirteenth, twelfth, or eleventh point of  $G(2)$ , this prescription brings  $\Delta$  to 0.0030, 0.0030, and 0.0025, respectively. One may try this for  $d=3$ .

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## APPENDIX A

We will present here, as an illustrative example, the calculation of  $\langle H_{0134} \rangle$ , where  $H_{0134}$  is the product of spins around an elementary plaquette. We will work in the transfer matrix formalism.<sup>(9)</sup> One first views the  $x$  and  $y$  directions as space and time directions. One row is arbitrarily chosen as the zero time row. At the sites on this row, labeled by integer  $n$ , one assigns matrices  $\sigma_i(n)$ ,  $i=1, 2, 3$ , obeying the Pauli algebra. Matrices at different sites commute. In terms of these a transfer matrix is defined:

$$T = \exp \left[ K \sum \sigma_3(n) \sigma_3(n+1) \right] \exp \left[ K^* \sum \sigma_1(n) \right] \quad (\text{A1})$$

where the sum is over the sites of the zeroth row and  $K=K_1$  and  $K^* = -\ln(thK)/2$ . The partition function is

$$Z = \text{Tr}(T^R) \quad (\text{A2})$$

where  $R$  is the number of rows. In the limit  $R \rightarrow \infty$  this simplifies to

$$Z = \langle 0 | T^R | 0 \rangle = t_{\max} R \quad (\text{A3})$$

where  $t_{\max}$  is the largest eigenvalue of  $T$  and  $|0\rangle$  the corresponding eigenvector. The thermal average of classical spins  $\langle s(n_1, y_1) \cdots s(n_k, y_k) \rangle$  is given by

$$\langle s(n_1, y_1) \cdots s(n_k, y_k) \rangle = \langle 0 | \tau [\sigma_3^{y_1}(n_1) \cdots \sigma_3^{y_k}(n_k)] | 0 \rangle \quad (\text{A4})$$

where

$$\sigma_3^y(n) = T^{-y} \sigma_3(n) T^y \quad (\text{A5})$$

and the time-ordering symbol  $\tau$  requires that the operators in square brackets be ordered such that  $y$  increases as we go from right to left.

Applying Eq. (A4) to the plaquette terms we get

$$\langle H_{0134} \rangle = \langle s_0 s_1 s_3 s_4 \rangle = \langle 0 | \sigma_3^1(0) \sigma_3^1(1) \sigma_3(0) \sigma_3(1) | 0 \rangle \quad (\text{A6})$$

Let us now use

$$\sigma_3^1(n) = T^{-1} \sigma_3(n) T = [C^* - S^* \sigma_1(n)] \sigma_3(n) \quad (\text{A7})$$

where  $C^*$  and  $S^*$  are  $Ch(2K^*)$  and  $Sh(2K^*)$  respectively. Now we use  $(\sigma_3)^2 = 1$ , to get

$$\begin{aligned} \langle H_{0134} \rangle &= \langle 0 | [C^* - S^* \sigma_1(1)] [C^* - S^* \sigma_1(0)] | 0 \rangle \\ &= C^{*2} - 2C^* S^* \langle | \sigma_1(0) | 0 \rangle + S^{*2} \langle | \sigma_1(0) \sigma_1(1) | 0 \rangle \end{aligned} \quad (\text{A8})$$

One now introduces the Clifford operators defined by

$$\begin{aligned} \Gamma_{n-1/2, n} &= \left[ \prod_0^{n-1} \sigma_1(m) \right] \sigma_3(n) \\ \Gamma_{n, n+1/2} &= \left[ \prod_0^{n-1} \sigma_1(m) \right] \sigma_2(n) \end{aligned} \quad (\text{A9})$$

obeying the anticommutation relations:

$$\{ \Gamma_a, \Gamma_b \} = 2\delta_{ab} \quad (\text{A10})$$

In terms of these,

$$\begin{aligned} \langle H_{0134} \rangle &= C^{*2} + 2iC^* S^* \langle 0 | \Gamma_{-1/2, 0} \Gamma_{0, 1/2} | 0 \rangle \\ &\quad - S^{*2} \langle 0 | \Gamma_{-1/2, 0} \Gamma_{0, 1/2} \Gamma_{1/2, 1} \Gamma_{1, 3/2} | 0 \rangle \end{aligned} \quad (\text{A11})$$

We now turn to Eq. (108) of Itzykson<sup>(9)</sup> to get the  $\Gamma\Gamma$  correlations. (He gives the expectation value of the  $\tau$  ordered products. These become

ordinary products for the equal time case we are considering). For the four  $\Gamma$  correlations, we use Wick's theorem:

$$\begin{aligned} \langle 0 | \Gamma_i \Gamma_j \Gamma_k \Gamma_l | 0 \rangle &= \langle 0 | \Gamma_i \Gamma_j | 0 \rangle \langle 0 | \Gamma_k \Gamma_l | 0 \rangle \\ &+ \langle 0 | \Gamma_i \Gamma_l | 0 \rangle \langle 0 | \Gamma_j \Gamma_k | 0 \rangle - \langle 0 | \Gamma_i \Gamma_k | 0 \rangle \langle 0 | \Gamma_j \Gamma_l | 0 \rangle \end{aligned} \quad (\text{A12})$$

Finally we need to take the  $K$  derivative of Eq. (A11) and isolate the  $\ln \delta$  part. This is readily done upon keeping upto order  $\delta^2$  terms in the integrals for the correlation functions given in Itzykson. [If we differentiate (A12) using the chain rule, the term that is not being differentiated must be evaluated exactly at  $\delta=0$ . These integrals can be reduced to Bessel functions. One uses the formula

$$(a - \cos x - \cos y)^{-1} = \int_0^\infty dt \exp[-t(a - \cos x - \cos y)]$$

which is valid for  $a > 2$ .]

Finally we must include the multiplicity factor, and drop a factor of  $-8/\pi$  to get the coefficient  $g_{0134}$ .

The 13 terms we considered involved four  $\Gamma$  correlators. The fourteenth term of Gupta and Corderey for which we did not calculate the coefficient  $g_{14}$  involved six  $\Gamma$  correlations. This fact, plus the fact that  $g_{14}$  could be reliably estimated to be  $\simeq 3$  (using scaling) and that  $g_{14}k_{14} \simeq 0.001$  explains our not computing it exactly.

### APPENDIX B

To get the curvature effects we needed the  $\ln \delta$  singularity in  $\partial^2 f' / \partial k_2^2$ . This quantity is not available in any published work. We will sketch its computation. The strategy will be to compute  $\partial^2 f / \partial k_2^2$  and then take the  $K_1$  derivative afterwards. Now

$$\begin{aligned} \partial^2 f / \partial K_2^2 &= 1/N \left[ \sum_{xy} \sum_{x'y'} (\langle H(x, y) H(x', y') \rangle - \langle H(0, 0) \rangle^2) \right] \\ &= \sum_{x,y} (\langle H(0, 0) H(x, y) \rangle - \langle H(0, 0) \rangle^2) \end{aligned} \quad (\text{B1})$$

where  $H(x, y)$  is the nnn coupling at site  $x, y$ . (There are two terms per site in  $H$ ;  $s_0 s_4$  and its reflection on the  $x$  axis.)

Consider first  $\langle H(0, 0) \rangle$ . We can write it as

$$\begin{aligned} \langle H(0, 0) \rangle &= \langle 0 | \sigma_3^{\frac{1}{2}}(1) \sigma_3^{\frac{1}{2}}(0) | 0 \rangle + \langle 0 | \sigma_3(0) \sigma_3^{-1}(1) | 0 \rangle \\ &= \langle 0 | \Omega(0, 0) | 0 \rangle \end{aligned} \quad (\text{B2})$$

In terms of this  $\Omega$  we can write

$$\langle H(0, 0) H(x, y) \rangle = \langle 0 | \tau \Omega(0, 0) \Omega(x, y) | 0 \rangle \tag{B3}$$

as long as  $x, y$  is not on the same row as  $(0, 0)$  and  $\text{mod}(x)$  is not less than or equal to 1. For these contact terms there is a problem because the  $\tau$  symbol treats  $\Omega$  as a block whereas the correct  $\tau$  ordering must be done with respect to the four  $\sigma_3$ 's (with four time coordinates) that occur in  $\Omega(0, 0) \Omega(x, y)$ . Assuming that these dangerous terms are treated with care, a typical term will be like

$$\langle 0 | \tau [\Gamma_0 \Gamma'_0 \Gamma'_{x,y} \Gamma'_{x,y}] | 0 \rangle$$

where  $\Gamma_0$  and  $\Gamma'_0$  are  $\Gamma$ 's centered near the origin while the other two are centered near  $x, y$ . If we now use Wick's theorem, the term  $\langle \Gamma_0 \Gamma'_0 \rangle \langle \Gamma'_{x,y} \Gamma'_{x,y} \rangle$  becomes equal to  $\langle L_0 \Gamma'_0 \rangle^2$  (by translation invariance). This term is exactly cancelled by the  $\langle 0 | \Omega(0, 0) | 0 \rangle^2$  term. The other two terms will have  $x, y$  dependence. Thus we will need terms like

$$\sum_{xy} \langle 0 | \Gamma_0 \Gamma'_{x,y} | 0 \rangle \langle 0 | \Gamma'_0 \Gamma'_{x,y} | 0 \rangle$$

Since the  $\Gamma\Gamma$  correlations are given as Fourier transforms anyway, what we want is then a convolution of the form

$$\int d^2q / (2\pi)^2 \Gamma\Gamma'(q) \Gamma'\Gamma(-q)$$

These are then evaluated, amends are made for the contact terms referred to earlier, the  $\ln \delta$  term is pulled out and finally, an overall factor of  $-8/\pi$  is dropped.

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