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Monte Carlo renormalization-group analysis of the classical Heisenberg model in two dimensions

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Monte Carlo renormalization-group methods were applied to the classical three-component Heisenberg model on a two-dimensional lattice. Expectation values of local correlations of spins and various sized block spins were computed using traditional Monte Carlo methods. By matching quantities at different length scales generated by different Monte Carlo Hamiltonians we directly determined the renormalization of the nearest-neighbor coupling. Using these data and the results of high-temperature expansions and low-temperature renormalization-group calculations we have determined that this model does not have a phase transition. We have also obtained the amplitude for the low-temperature divergence of the susceptibility and the correlation length.

I. INTRODUCTION

The renormalization group (RG) has developed in recent years into a powerful technique for studying the critical behavior of statistical mechanical systems. The blending of block-spin RG ideas with Monte Carlo (MC) techniques by Ma[1] and Swendson[2] has greatly increased the versatility of these methods.

A statistical mechanical problem of particular interest to high-energy theorists is the four-dimensional non-Abelian lattice gauge theory, which so far has resisted all attempts at analytic solution. Wilson[3] has implemented a MCRG scheme particularly suited to this model, where a smooth crossover from the small fluctuation to large fluctuation regime is expected. His calculations are currently underway.

In this paper we apply Wilson's version of the Ma and Swendson ideas to the two-dimensional (2D) n-component classical Heisenberg model (specifically $n=3$) where a similar smooth crossover is expected. Our purpose is twofold. First, we hope to describe the behavior of this model quantitatively in all regimes, and, second, we hope to demonstrate the validity of the MCRG techniques in this relatively simple situation, opening the way for their application to other more complicated systems.

II. CLASSICAL HEISENBERG MODEL

The 2D n-component Heisenberg model is defined by the partition function

$$Z=\sum_{|\vec{S}|=1}\exp\left(\frac{1}{T}\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j\right), \tag{1}$$

where $\vec{S}$ is an n-component unit vector, T is the temperature in dimensionless units, and $\langle ij\rangle$ denotes nearest-neighbor sites on a square lattice.

When $n=1$ this model reduces to the 2D Ising model, known to have a phase transition between a disordered high-temperature phase with exponentially decaying correlations and a low-temperature magnetized phase. At $n=2$ this model is the 2D planar model, which behaves according to the Kosterlitz-Thouless [4] theory which predicts a phase transition between a high-temperature phase with exponentially decaying correlations and a low-temperature phase with power-law decay. As n approaches ∞ this model becomes the spherical model,[5] known to have exponentially decaying correlations for all nonzero T. We are interested in the intermediate region $2<n<\infty$, and in particular would like to know for what value of n a phase transition ceases to occur.

Real progress in answering this question first came with Polyakov's[6] development of a low-temperature renormalization group, further elaborated on by Brezin and Zinn-Justin[7] and Nelson and Pelkovitz.[8] At low T one assumes the spins are almost aligned. One can then do a spin-wave expansion; we write

$$\vec{S}=[\pi_1,\pi_2,\ldots,\pi_{n-1},(1-\pi_a\pi_a)^{1/2}], \tag{2}$$

where a sum on a ($a=1,2\cdots n-1$) is implied. Assuming the π fields are small (formally of order $\sqrt{T}$), we expand the nonlinearities of the square root and the integration measure to do a perturbative analysis in T.

Following the spirit of Wilson's renormalization group,[9] we can integrate out the high-momentum modes of the π field, and rescale our units of length

and our fields to obtain a new system with the same form of interaction as before, but at a different temperature. If we integrate our momenta between Λ and Λ/b (where Λ is the high-momentum cutoff), we find

$$\frac{dT}{d\ln b} = -(d-2)T + \frac{(n-2)}{2\pi}T^2 + \frac{(n-2)}{(2\pi)^2}T^3 + O(T^4) \ . \tag{3}$$

We often use the variable $K = 1/T$, in terms of which Eq. (3) becomes

$$\frac{dK}{d\ln b} = (d-2)K - \frac{(n-2)}{2\pi} - \frac{(n-2)}{(2\pi)^2}\frac{1}{K} + O\left[\frac{1}{K^2}\right] \ . \tag{4}$$

These remarkable formulas tell us a great deal about the behavior of the system. Note first that for $d > 2$ the right-hand side of Eq. (3), called the β function in field theory, vanishes at some $T = T_c$. If the function vanishes, then the system is invariant under length rescaling, and so all lengths characteristic of the system must be either zero or infinite. In fact, the correlation length at T_c is infinite; thus T_c is a critical point of the system. The critical exponents can be read off Eq. (3) by calculating the slope of the β function at T_c.

In two dimensions a very interesting phenomenon occurs. For $n > 2$ the β function is always positive, so no matter how low a T we start with, the system iterates upon repeated rescaling to higher and higher temperatures, eventually leaving the domain of validity of Eq. (3). If we imagine for a moment that Eq. (3) is qualitatively correct for all T, we can say that the system always iterates to a regime where high-temperature expansions, indicating exponetially decaying correlations, are valid. So the system would be disordered at any $T > 0$ for all $n > 2$.

What makes this behavior particularly interesting is that a formula very similar to Eq. (3) holds in non-Abelian gauge theories.[10] T is replaced by g^2, the coupling constant of the theory, $(d-2)$ is replaced by $(d-4)$, and the numerical factors are changed. When translated, the above analysis would imply that non-Abelian gauge theories are disordered for all g^2 in $d = 4$. The disordered behavior of a gauge theory means confinement of static sources. The assertion then is that non-Abelian gauge theories confine for all couplings at $d = 4$. It is very important to discover if this is indeed the way gauge theories behave. The 2D Heisenberg system, then, takes on new importance as an analogous system in which to explore such questions.

In order to decide if the model is really disordered for all T, we must be able to extend our understanding of the low-T regime described by Eq. (3). We require some technique that can take us from the low-temperature regime to the high-temperature regime, allowing us to demonstrate that there are no intervening pathologies and to calculate quantitatively the behavior of the model.

In Secs. III–V we describe an approach for attacking this problem.

III. BLOCK-SPIN RENORMALIZATION GROUP VIA MONTE CARLO

The block-spin renormalization-group (RG) method is not in principle restricted to a perturbative regime. This method was first formulated by Kadanoff[11] and later made a working tool by Niemeijer and van Leeuwen.[12] It has been extensively applied to various discrete spin systems.

We can easily construct such an RG for the 2D Heisenberg system. Consider the original lattice of spins. Group each four-site square of spins into a block spin (Fig. 1) and define a block-spin variable $\vec{t}$ as follows:

$$\vec{t}_{n'} = \sum_{j\in n'} \vec{S}_j \Big/ \left\| \sum_{j\in n'} \vec{S}_j \right\| \ , \tag{5}$$

where the $\vec{S}_i$ are the original spins, n' denotes a site on the block lattice, and $j \in n'$ labels the four sites within block n'. Note that the lattice spacing of the block lattice is twice that of the original lattice.

We now define a new system whose degrees of freedom are the block spins $\vec{t}$. Let

$$e^{\mathcal{H}'(\{\vec{t}\})} = \int_{\{\vec{S}\}} K(\{\vec{S}\},\{\vec{t}\}) e^{\mathcal{H}(\{\vec{S}\})} \ , \tag{6}$$

where

$$K(\{\vec{S}\},\{t\}) = \prod_{n'} \delta\left(t_{n'} - \sum_{j\in n'} \vec{S}_j \Big/ \left\| \sum_{j\in n'} \vec{S}_j \right\| \right) \ , \tag{7}$$

where $\mathcal{H}$ is the Hamiltonian of the original system and $\mathcal{H}'$ is the new Hamiltonian of the block spins. This is the RG transformation.

There are several important properties of the transformation [Eq. (6)]: (i) The partition function is unchanged. This is demonstrated by integrating both sides of Eq. (6) over the $\vec{t}$ spins. The left-hand side is just the partition function of the block system. The integral over the δ function gives 1 and the

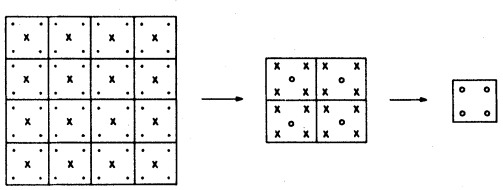

FIG. 1. Schematic diagram of block-spin procedure.

right-hand side then becomes the partition function of the original system.

(ii) The correlation length of the block spins in units of the block lattice spacing is one-half that of the original spins in units of the original lattice spacing. This rescaling of lengths is the key to any RG transformation.

(iii) The block Hamiltonian will in general contain many new interactions, even if the original $\mathcal{H}$ contains only one. Next-nearest neighbor, second-nearest neighbor, four-spin coupling, etc., will in general all be generated.[12] The luxury of tracking the effect of renormalization by following only one coupling, as in Eq. (3), is restricted to the low-temperature perturbation regime.

(iv) Even on a quite small lattice, say 4×4, the evaluation of Eq. (6) is a formidable task, involving an integral over a very large dimensional space (e.g., 32D for $n=3$ on a 4×4 lattice). Since no analytical tricks have yet appeared, the only alternative is a numerical evaluation, and the direct numerical evaluation of Eq. (6) would be very difficult. Fortunately a method exists for dealing with a calculation like this, the Monte Carlo technique.

The Monte Carlo (MC) method generates a sequence of spin configurations distributed according to the Boltzmann distribution $e^{\mathcal{H}[\vec{S}]}/Z$. In principle any thermodynamic quantity or correlation function can be computed using MC. However, for quantities sensitive to long-wavelength fluctuations, one must do MC on a lattice large enough to represent these long-wavelength fluctuations accurately. Thus, the lattice should be somewhat larger than the correlation length. Near criticality correlation lengths are huge, and the required lattices are computationally impractical. We can circumvent this difficulty by combining MC with block-spin RG.

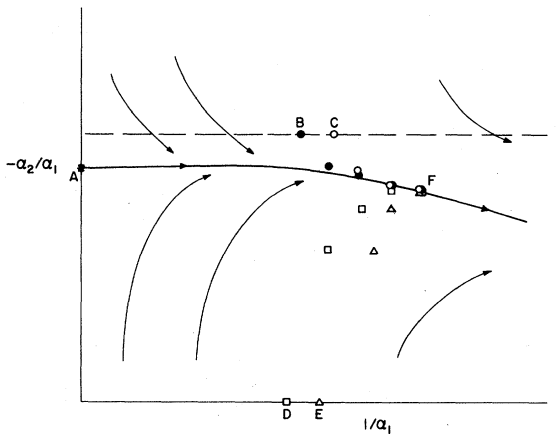

FIG. 2. Possible diagram of renormalization-group flows. Point A represents the low-temperature fixed point. B, C, D, and E represent possible starting points for the iteration of the MCRG procedure. α_1 and α_2 are coupling constants in the Hamiltonian which are proportional to $1/T$.

Ma[1] and Swendson[2] made the following observation: if one generates a sequence of configurations $\{\vec{S}\}_i$ distributed according to $e^{\{S\}}/Z$ and to each of these configurations applies the blocking rule [Eq. (5)] to generate a sequence of block-spin configurations $\{\vec{t}\}_j$, *then* the $\{\vec{t}\}_i$ are, by Eq. (6), distributed according to $e^{\mathcal{H}'\{\vec{T}\}}/Z$. (Recall that Z is the same for both systems.) Thus it is easy to compute block-spin expectation values by Monte Carlo. Block-spin expectation values do not directly reveal the couplings of the block-spin Hamiltonian, but can be used to determine if two Hamiltonians have the same couplings. So an admittedly impractical scheme for determining the block Hamiltonian couplings would be to simulate systems with many coupling constants and adjust these by trial and error to match the calculated block expectation values. Searching the many-parameter space required, however, is computationally unmanageable. However, we expect from the low-temperature analysis that all but one combination of interactions is irrelevant.[13] That is, after repeated iterations all Hamiltonians in some neighborhood of the $T=0$ fixed point collapse into a one-dimensional submanifold of interaction space. This line is called the "renormalized trajectory" (RT). If we could iterate by Monte Carlo enough times to reach the RT, then we need only parametrize our location in this one-dimensional space.

We depict the expected situation schematically in Fig. 2, where α_1 and α_2 are two representative couplings; both are proportional to $1/T$. We emphasize that this picture is a two-dimensional projection of the infinite-dimensional parameter space. Point A is the unstable fixed point at $T=0$ implied by Eq. (3).

We now describe how to use the Monte Carlo renormalization group (MCRG). Initially we do not know where the RT is, but suppose we could draw a line (e.g., the dashed lined in Fig. 2) not too far from it, say a line where a small number of iterations would carry us onto the RT. We could then do the following: start at some point on our line, e.g., point B of Fig. 2. Iterate (the filled circles), arriving close to the RT after one jump and then continue along it. (In what follows we refer to a trajectory by its point of origin.) Now search our line for a point C such that after one iteration (the open circles) it reaches the RT at close to the same location that B did after two iterations and continues to track B. We check how close these points are by comparing various block expectation values. At point F, for example, the B system blocked 4 times and C blocked 3 times have almost the same Hamiltonian. Hence, they will have almost the same correlation length ξ. But we iterated 4 times from B to get to F so B has correlation length $2^4\xi$. Similarly, point C has correlation length $2^3\xi$. So B has twice the correlation length of C. We have computed the shift (the distance BC)

needed to change the correlation length by a factor of 2. We are therefore computing the β function for the model along our line!

If we want information along the $\alpha_2=0$ axis, we can begin with a point there, such as D, and iterate it until it approaches the RT. (In general, this will take more iterations than from our carefully chosen line.) Once we have matched onto a point on the RT we can transfer information back to the $\alpha_2=0$ axis. If we can perform the required number of iterations, we can compute the β function directly along the $\alpha_2=0$ axis by finding a point such as E. If T_1 and T_2 parametrize distance along any two lines in coupling space, then it is a consequence of the low-temperature RG that points with equal correlation length are characterized

$$T_1 = T_2 + cT_2^2 + O(T_2^3) \ . \tag{8}$$

(We assume suitable normalizations.) From Eq. (3) we see that the β function is identical through $O(T^3)$ along the two lines. This result allows us to use Eq. (3) to calculate the β function along *any* line at low temperature.

We can repeat the procedure outlined above, obtaining a sequence of points with correlation lengths differing by a factor of 2 until we are at a temperature T large enough that we can calculate the correlation length of the system directly by direct MC or high-temperature expansions. We then can compute the correlation length of any point on our path by counting the number of points at which a jump by a factor of 2 occurs between this initial point and the high-temperature point.

This procedure, if it worked as described, would confirm *a posteriori* that the situation is as depicted in Fig. 2 (at least in the neighborhood of our line). Other possibilities, such as *two* relevant operators, would make the matching fail. A nontrivial fixed point close to our line would show up as a point that matched onto itself.

There is no guarantee that the situation is as depicted in Fig. 2. In particular we cannot be certain that the RT will retain its attractive character all the way to the high-T regime. The only way to tell is to try it.

Before we proceed, we must discuss a complication of comparing quantities calculated on a finite lattice. If one computes various expectation values of identical Hamiltonians on different size lattices, the numbers will differ. The size of the difference will depend on the range of the operator compared to the size of the lattice. So in comparing sets of expectation values to see whether they come from the same Hamiltonian we must make sure they are computed on the *same size* lattice. If we take point B (Fig. 2) on a 32×32 lattice and block it twice, we get a block-spin Hamiltonian on an 8×8 lattice. To find a point C that matches, we could take a 16×16 lattice and block it once to get an 8×8 lattice. We could then compare the expectation values of the two 8×8 lattices. If they agree, they have the same Hamiltonian.

IV. CALCULATION

A. Low-temperature analysis

In order to test the method outlined in Sec. III we must choose some line which we think will not be too far from the RT. One possibility, suggested by the low-temperature RG, is to find a set of couplings close to the $T=0$ fixed point and hold their ratios fixed as we move away from it. To find this set of couplings, we study the RG transformation [Eq. (6)] at low T within the (lowest-order) spin-wave approximation.

It is impractical to keep a large number of couplings in the computer calculation, so we somewhat arbitrarily decided to keep just three (nearest, next-nearest, and third-nearest neighbor) and to get as close as possible to the low-T fixed point with them. Our $\mathcal{H}$ looks like

$$\mathcal{H} = K_1 \sum_{n,\hat{\mu}} \vec{S}_n \cdot \vec{S}_{n+\hat{\mu}} + K_2 \sum_n (\vec{S}_n \cdot \vec{S}_{n+\hat{x}+\hat{y}} + \vec{S}_n \cdot \vec{S}_{n+\hat{x}-\hat{y}}) + K_3 \sum_{n,\hat{\mu}} \vec{S}_n \cdot \vec{S}_{n+2\hat{\mu}} \ , \tag{9}$$

where n is a lattice site and $\hat{\mu}$ a unit vector in the lattice. For the spin-wave calculation it is convenient to regroup these terms in a "continuum" formulation

$$-\mathcal{H} = \sum \{ \alpha_1 (\nabla_\mu \vec{S}_n) \cdot (\nabla_\mu \vec{S}_n) + \alpha_2 (\nabla_\mu \nabla_\mu \vec{S}_n) \cdot (\nabla_\nu \nabla_\nu \vec{S}_n) + \alpha_3 [(\nabla_x^2 \vec{S}_n) \cdot (\nabla_x^2 \vec{S}_n) + (\nabla_y^2 \vec{S}_n) \cdot (\nabla_y^2 \vec{S}_n)] \} \ , \tag{10}$$

where

$$\nabla_\mu f_n = f_{n+\hat{\mu}} - f_n \ .$$

We have

$$K_1 = 2\alpha_1 + 16\alpha_2 + 8\alpha_3 \ , \quad K_2 = -4\alpha_2 \ , \quad K_3 = 2\alpha_2 - 2\alpha_3 \ . \tag{11}$$

Because the α_2 and α_3 terms contain more derivatives, we expect them to be irrelevant operators around the $T=0$ fixed point.

TABLE I. Spin-wave results. $NN = \alpha_1(1 - C_{NN})$ and $NNN = \alpha_1(1 - C_{NNN})$. C_{NN} and C_{NNN} are defined in Sec. IV B.

	32×32 lattice			16×16 lattice	
Block length	NN	NNN	Block length	NN	NNN
		$\alpha_1:\alpha_2:\alpha_3 = 1:0:0$			
1	0.2498	0.3178			
2	0.1618	0.2172	1	0.2490	0.3163
4	0.1341	0.1846	2	0.1589	0.2115
8	0.1153	0.1560	4	0.1220	0.1630
16	0.0598	0.0840	8	0.0616	0.0859
		$\alpha_1:\alpha_2:\alpha_3 = 5:1:0$			
1	0.1464	0.2037			
2	0.1275	0.1805	1	0.1457	0.2023
4	0.1238	0.1739	2	0.1245	0.1748
8	0.1125	0.1531	4	0.1116	0.1523
16	0.0591	0.0832	8	0.0588	0.0830
		$\alpha_1:\alpha_2:\alpha_3 = 5:2:0$			
1	0.1077	0.1554			
2	0.1082	0.1579	1	0.1069	0.1539
4	0.1160	0.1653	2	0.1053	0.1521
8	0.1100	0.1505	4	0.1038	0.1438
16	0.0584	0.0825	8	0.0564	0.0805

To see how close we are to a fixed point, we examine various expectation values and see how much they change upon iteration. We computed nearest-neighbor (NN) and next-nearest-neighbor (NNN) spin-spin correlations for different block sizes in the spin-wave approximation. This just involves doing some Gaussian integrals. The required k-space sums were done on the computer. Results for three α_1, α_2, α_3 values are displayed in Table I.

It is clear that the $\alpha_1:\alpha_2:\alpha_3 = 5:1:0$ Hamiltonian is closer to a fixed point than either of the others. We work with this set of ratios, but make no special claims for it. Undoubtedly others would work as well.

We now turn to the actual Monte Carlo calculation.

B. Monte Carlo calculation

We used the traditional Metropolis MC procedure to generate spin configurations located on a square lattice with periodic boundary conditions. Spins were updated by adding to them a random vector selected out of a sphere of diameter $d_{\max}$ and then normalizing the spin vector. This updating procedure satisfies the symmetry requirement of the Metropolis method. It is commonly believed that $d_{\max}$ should be adjusted to give an acceptance ratio of 0.5; however, we have found that at low temperatures better statistics can be obtained with lower acceptance ratios.

We selected five quantities to compute for each block size

$$C_{NN} = \langle \vec{S}_n \cdot \vec{S}_{n+\mu} \rangle \ , \tag{12a}$$

$$C_{NN2} = \langle (\vec{S}_n \cdot \vec{S}_{n+\mu})^2 \rangle \ , \tag{12b}$$

$$C_{NNN} = \langle \vec{S}_n \cdot \vec{S}_{n+\mu+\nu} \rangle, \quad \mu \neq \nu \ , \tag{12c}$$

$$C_{NNN2} = \langle (\vec{S}_n \cdot \vec{S}_{n+\mu+\nu})^2 \rangle, \quad \mu \neq \nu \ , \tag{12d}$$

$$C_{4S} = \langle (\vec{S}_n \cdot \vec{S}_{\mu+\nu})(\vec{S}_{n+\mu} \cdot \vec{S}_{n+\mu+\nu}) \times (\vec{S}_{n+\mu+\nu} \cdot \vec{S}_{n+\mu})(\vec{S}_{n+\mu} \cdot \vec{S}_n) \rangle \ . \tag{12e}$$

These quantites are the ones we use to ascertain if two Hamiltonians are close to each other. In addition we always calculated the susceptibility $\chi \equiv (1/N) \times \langle (\sum_n \vec{S}_n)^2 \rangle$ and sometimes the spin-spin correlation function $C(n) = \langle \vec{S}_0 \cdot \vec{S}_n \rangle$.

In analyzing MC data it is important to be able to estimate errors correctly. In particular, we must determine how many statistically independent samples we have from a given MC run. Configurations that differ by only one pass through the lattice will not be independent of each other unless $d_{\max}$ is very large and the temperature is very high. In general, configurations are correlated over many passes and

one must take this into account in computing standard deviations σ. We do this by grouping numbers into groups of L numbers, averaging them and then computing the σ of the groups. When σ drops by $1/\sqrt{L}$ on grouping we believe we have independent samples and call the number of passes within an independent sample the correlation time τ. The error for a particular quantity is then the σ of the independent samples divided by $\sqrt{L}$.

τ depends on $d_{\max}$, the temperature and the quantity being studied. Large block quantities have larger τ's than small block ones. In the regime we studied τ ranged from 200 to 1300 passes for the 16×16 block averages on the 32×32 lattice. τ was usually less than 400 passes for the 8×8 block average on the 16×16 lattice.

At low temperatures τ can be cut down significantly by using a low-acceptance ratio. For example at $\alpha_1=0.7$, τ can be reduced by a factor of around 4 by reducing the acceptance ratio from 0.5 to 0.3. This means the same accuracy can be achieved in one-fourth the computer time.

Because of these correlations we compute averages once every eight passes. This saves computer time with a negligible loss in statistics (except, perhaps, at the highest temperatures).

Our program was run on an array processor manufactured by Floating Point Systems, Inc. This inexpensive source of computing power made this calculation feasible. The update time for the three-coupling Hamiltonian is about 0.5 and about 0.4 msec for the one-coupling Hamiltonian. This rather slow time could be improved by a factor of 3–6 by coding the inner loops of the program in assembly language rather than using the Cornell FORTRAN compiler. The random number generator needed for the spin updating was written in assembly language and contributed a negligible amount of time to the calculation.

To compute our matching quantities we made runs ranging from 30 000 to 200 000 passes through the lattice. We routinely discarded approximately the first 20% of a run to allow for equilibrium.

V. RESULTS

A. Nearest-neighbor correlation

Before proceeding to our MCRG results we discuss the behavior of the nearest-neighbor correlation, C_{NN}. In Fig. 3 the Monte Carlo data for one-coupling constant calculations ($K_1=K$, $K_2=0$, $K_3=0$) are shown along with the high-temperature series (HT)[14] to order K^{10} and the low-temperature spin-wave (SW) calculation to lowest order, i.e., the equipartition theorem. The units are chosen so that $C_{NN}=1$ when the spins are perfectly aligned.

The high-temperature MC data points have an uncertainty of a few tenths of a percent and agree within this uncertainty with the HT series up to around $K=1.4$. In addition to showing where the series breaks down, this is an excellent test of our MC calculations.

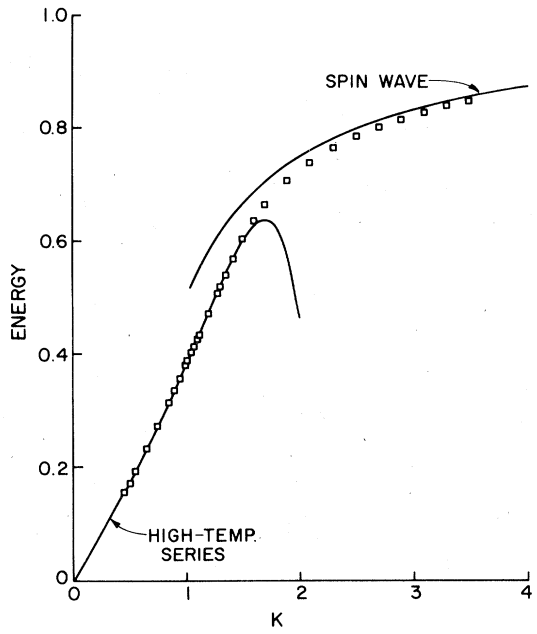

FIG. 3. Energy vs K. The uncertainty in the data is smaller than the size of a square.

The MC points shown in Fig. 3 beginning at around $K=2.0$ are just below the SW results, as would be expected since we are not yet at very low temperatures, where the lowest order SW result is sufficiently accurate. At lower temperatures (not shown) the SW and MC data agree as expected.

By comparing the MC data with the analytic results we see that the crossover region between HT and SW calculations occurs in the region around $K=1.3-2.0$. Also, we note that the C_{NN} curve is rather featureless. This behavior may not, however, be relevant to the critical properties of the system. For example, the equivalent curve in the $n=2$ planar model exhibits similar behavior despite the occurrence of the Kosterlitz-Thouless phase transition.

B. MCRG data

We now wish to present the new data calculated using MCRG. First we must be confident that the procedure outlined above actually works. An example of a typical match is shown in Table II for a pair of three coupling constant Hamiltonians matching a 32×32 lattice into a 16×16 lattice. As can be seen, the two largest block sizes match well within the uncertainties of the data. The next length scale (i.e., 4×4 blocks on the 32×32 lattice and 2×2 on

TABLE II. Representative MCRG match of two three-coupling Hamiltonians. The last two length scales match within one σ, and the third largest scales differ by about one σ. The 32×32 lattice was run through about 133 000 passes and the 16×16 lattice about 106 000 passes through the lattice.

Block length	C_{NN}	C_{NN2}	C_{NNN}	C_{NNN2}	C_{4S}
		32×32 lattice $\alpha_1 = 0.70$			
1	0.7817	0.6560	0.7030	0.5669	0.3962
σ	0.0002	0.0002	0.0003	0.0003	0.0003
2	0.7888	0.6620	0.7084	0.5714	0.4079
σ	0.0007	0.0008	0.0012	0.0012	0.0012
4	0.7727	0.6422	0.6889	0.5531	0.3796
σ	0.0019	0.0023	0.0033	0.0031	0.0032
8	0.7680	0.6369	0.6929	0.5571	0.3713
σ	0.0057	0.0058	0.0096	0.0092	0.0099
16	0.8597	0.7573	0.8083	0.6865	0.5564
σ	0.0094	0.0136	0.0165	0.0203	0.0212
		16×16 lattice $\alpha_1 = 0.640$			
1	0.7608	0.6324	0.6757	0.5417	0.3615
σ	0.0003	0.0003	0.0005	0.0004	0.0004
2	0.7694	0.6391	0.6845	0.5845	0.3743
σ	0.0009	0.0010	0.0015	0.0014	0.0015
4	0.7670	0.6359	0.6882	0.5526	0.3701
σ	0.0022	0.0026	0.0036	0.0035	0.0037
8	0.8576	0.7548	0.8023	0.6787	0.5523
σ	0.0026	0.0039	0.0047	0.0065	0.0065

16×16) is about one standard deviation off from matching. It is clear that we could have all three scales match within one standard deviation by matching onto a 16×16 lattice at a slightly higher value of α_1. However, SW theory suggests that we have not quite iterated to the renormalized trajectory at this scale, so it is probably more reliable to use the 8×8 to 4×4 matching as the basis for determining the change in α_1. We have performed a number of matchings along this three-coupling path (i.e., $\alpha_1:\alpha_2:\alpha_3 = 5:1:0$).

Although this path is more useful than the one coupling path for the MCRG at low temperatures it is more difficult to study at high temperatures. In particular, the high-temperature expansion is more difficult to calculate. In order to join onto the high-temperature series results for one coupling we must find a correspondence between one- and three-coupling paths. At low temperatures this amounts to computing the constant c in Eq. (8). Comparing the 8×8 block-spin expectation values on a one-coupling lattice with that on a three-coupling lattice we found the correspondence to be (at $K = 1.50$ and 1.42)

$$2\alpha_1(\text{3-coupling}) + 0.42 \pm 0.02 = 2\alpha_1(\text{1-coupling}) \equiv K . \tag{13}$$

This K is the same as in Eq. (4). If the correspondence is a constant shift in $2\alpha_1$, as suggested by Eq. (8), our determination of the β function will not be affected by the uncertainty in determining the constant C.

Although spin-wave theory suggests that for one-coupling Hamiltonians we can only make an MCRG match on our largest length scale we have found numerically that at intermediate tempeatures we are able to match on two length scales. So we have performed a number of matches directly on one-coupling Hamiltonians.

In Fig. 4 we show the MCRG results for ΔK, which measures the change in K going from a lattice of correlation length ξ to one of $\frac{1}{2}\xi$. A positive ΔK

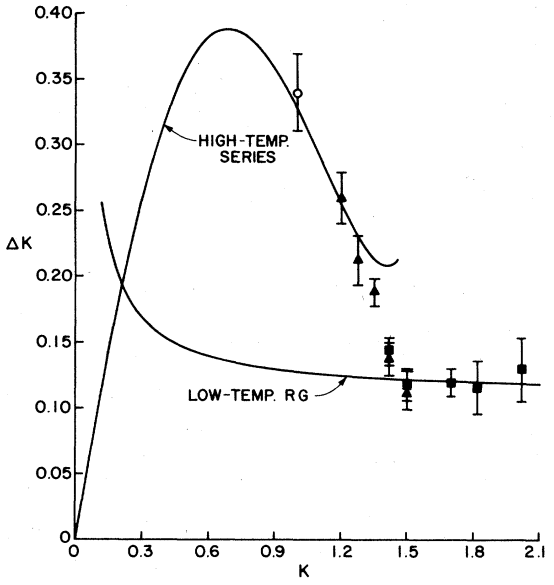

FIG. 4. ΔK vs K. ΔK is the change in K needed to go from a lattice with correlation length ξ (at K) to one of $\frac{1}{2}\xi$. The filled squares are MCRG data using three-coupling Hamiltonians, the filled triangles are MCRG data using one-coupling Hamiltonians, and the open circle is a MC direct calculation of ξ plus the high-temperature-series calculation of $\frac{1}{2}\xi$.

corresponds to a disordered phase.

The data points represent MCRG results for three- and one-coupling constant Hamiltonians matching 32×32 onto 16×16 and 16×16 onto 8×8 lattices. These results are listed in Table III. One point on the curve is based on calculating ξ directly from MC, because at this high temperature the MCRG procedure breaks down, as explained below. A high-temperature ΔK was computed from a ten-term series for ξ.[15] The other curve shown in the figure is the low-temperature RG result to two-loop accuracy.

The uncertainty of the data points is determined by multiplying the change in K as the block-spin averages change by the uncertainty in these quantities. In plotting the three-coupling results on this graph, we assume a constant shift between $2\alpha_1$ (three-coupling) and K of 0.42. The uncertainty in this shift results in some uncertainty in the position of these points along the K direction of the graph. If the shift is not constant there is an additional uncertainty added to ΔK. For example, at $\alpha_1=0.427$ (three-coupling) we find $\Delta K=0.164$ even though the corresponding one-coupling lattice at $K=1.28$ gives $\Delta K=0.21$. This indicates that at this temperature the shift is not constant. However, at $K=1.50$ and 1.42 the three-coupling results agree with the one-coupling results, indicating that the shift is constant within statistical uncertainties.

TABLE III. MCRG results. K is the nearest-neighbor coupling for one-coupling Hamiltonians, and $K\equiv2\alpha_1+0.42$ for three-coupling Hamiltonians, where α_1, α_2, and α_3 are defined by Eq. (10) and $\alpha_1:\alpha_2:\alpha_3=5:1:0$. ΔK is the change in K as one goes from a lattice of correlation length ξ to one of $\frac{1}{2}\xi$. The fourth column lists the side lengths of the two lattices used in computing ΔK.

K	No. of couplings	ΔK	Lattice
$n=3$			
2.02 ($\alpha_1=0.80$)	3	0.130 ± 0.025	$32\rightarrow16$
1.82 ($\alpha_1=0.70$)	3	0.116 ± 0.020	$32\rightarrow16$
1.70 ($\alpha_1=0.64$)	3	0.120 ± 0.010	$16\rightarrow8$
1.59[a] ($\alpha_1=0.585$)	3	0.060 ± 0.007	$08\rightarrow4$
1.50	1	0.112 ± 0.017	$32\rightarrow16$
1.50 ($\alpha_1=0.54$)	3	0.118 ± 0.011	$16\rightarrow8$
1.42	1	0.138 ± 0.014	$32\rightarrow16$
1.42[b] ($\alpha_1=0.50$)	3	0.146 ± 0.008	$32\rightarrow16$
1.35	1	0.189 ± 0.011	$32\rightarrow16$
1.28	1	0.216 ± 0.032	$32\rightarrow16$
1.28	1	0.209 ± 0.006	$16\rightarrow8$
1.274[a] ($\alpha_1=0.427$)	3	0.164 ± 0.004	$16\rightarrow8$
1.20	1	0.260 ± 0.020	$32\rightarrow16$
1.05[a]	1	0.265 ± 0.030	$32\rightarrow16$
$n=2$			
1.07 ($\alpha_1=0.325$)	3	0.025 ± 0.030	$32\rightarrow16$
1.20	1	-0.025 ± 0.020	$32\rightarrow16$
$n=6$			
9.42 ($\alpha_1=4.5$)	3	0.4	$32\rightarrow16$

[a]These points give anomalous values of ΔK for reasons cited in the text.

[b]The MC run used here was inadvertently computed with a spin update procedure utilizing a slight sampling bias. We have checked the 16×16 results for changes due to this bias and found them not detectable to our accuracy. Thus, we feel our value for ΔK is correct.

We have found that with a three-coupling Hamiltonian we could match 16×16 onto a 8×8 lattice on two length scales. We used the largest scale to actually determine the numerical value of ΔK. We also tried one low-temperature match of an 8×8 onto a 4×4 lattice and assumed that there was matching of the 4×4 onto 2×2 block averages. This gave a result for ΔK almost one-half that given by our other MCRG results and the low-temperature RG. We thus conclude that these lattices are not large enough relative to the range of the interactions generated by the block spin transformation to accurately represent it.

This procedure seems to break down at $K=1.05$.

When C_{NN}, C_{NNN}, and C_{4S} were matched we found that C_{NN2} and C_{NNN2} did not match by many standard deviations. We conclude that at this temperature the Hamiltonian does not iterate to the renormalized trajectory under our blocking procedure.

As a comparison test we tried our method on two planar model lattices. In this model one expects a line of critical points ($\Delta K = 0$) for $K > K_c$, where K_c is around 1.1. As can be seen from our data in Table III, the MCRG results are close to the expected $\Delta K = 0$. In fact, for the three-coupling Hamiltonian we may be slightly into the disordered phase, where we expect ΔK to be greater than 0. For the one-coupling result we may have a slight systematic error due to not having reached the renormalized trajectory. This effect tends to make ΔK too low. In any event, there is a dramatic distinction between the planar model data and that of the Heisenberg model.

In addition, we performed a qualitative check on the $n = 6$ component model at low T where we expect from the low-temperature RG that $\Delta K = 0.44$. We found $\Delta K \approx 0.4$, clearly distinct from the LT $n = 3$ model results.

Our MCRG results clearly join onto both the high- and low-temperature analytic results. The remarkable feature of these results is that the low-T RG is valid down to a correlation length of roughly five lattice spacings, a region which is within the scope of conventional Monte Carlo.

In principle we could test the low-T RG to very low temperatures, but in practice this is impossible because the various quantities used in the matching change very slowly with K and the correlation times are long. So incredibly long MC runs are necessary to achieve the very small σ needed to determine an accurate ΔK. Nevertheless, we have a ΔK good to around 20% at $K = 2.0$ where the correlation length is around 240 lattice spacings, a feat far beyond the capabilities of conventional MC.

C. Correlation length

In the region where correlation lengths are short enough to be computed by straight MC we can independently verify the MCRG results. There are various ways of extracting ξ from our data. One method consists of calculating the spin-spin correlation function and fitting it to a function with an exponentially decaying factor. One difficulty with this procedure is that the exact form of the spin-spin correlation function is not known and the ξ determined is sensitive to the approximation form chosen. In addition the answer depends somewhat on the range of r in $\langle S(0)S(r)\rangle$ used in the fit. Thus, we have only been able to determine ξ to ± 10–20%. Our values agree with the MCRG results within these uncertainties.

The second method for extracting ξ is to calculate the second moment of the spin-spin correlation function. The difficulty with this definition for MC implementation is that the weight of the second-moment peaks at 3ξ, so that the MC lattice must have a correlation length smaller than at least $\frac{1}{3}$ of the size of the system. In addition, the second moment gives a large weight to the large r part of the spin-spin correlation function, which is the least accurate part of the MC calculation. On the other hand, there is no ambiguity in extracting ξ from the second moment.

These MC results are shown in Fig. 5 along with the HT series result[15] and the low-temperature result, which is given by

$$\xi = C_0 e^{2\pi K}\left(\frac{1}{1+2\pi K}\right), \tag{14}$$

where we find from our MCRG and MC results that C_0 is around 0.010 with an uncertainty of around 30%. This uncertainty includes the MCRG uncertainties and also possible analytic corrections due to the third loop term in $\beta(K)$, assuming that the coefficient in front of this term is of the same order as that of the previous terms.

The actual nature of the joining between HT and LT is rather interesting. The breakaway from the low-temperature RG is very sharp. One speculation

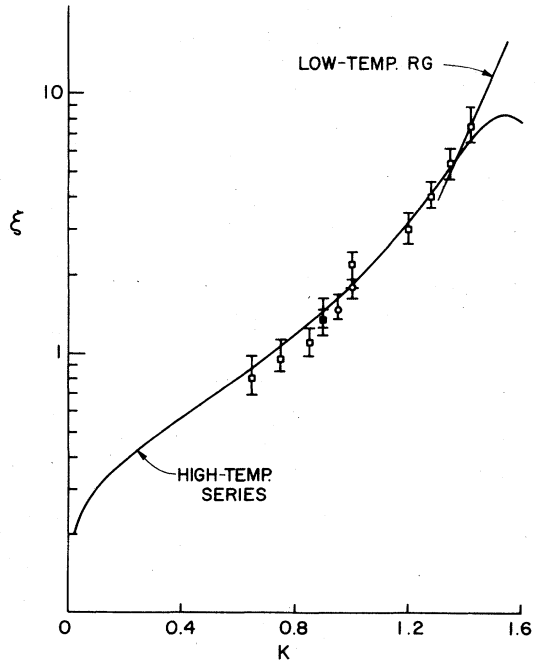

FIG. 5. Correlation length, ξ vs K. Squares are based on the asymptotic decay of the MC calculation of the spin-spin correlation function. The circles are based on a direct MC calculation of the second moment of the spin-spin correlation function. All data are from one-coupling Hamiltonians.

is that this behavior is due to instanton configurations becoming energetically important.[16] We have looked at graphical displays of spin configurations at equilibrium and found no obvious evidence of instantons. However, this is not conclusive since for the planar model it is also difficult to spot vortex configurations by eye, even though they are known to be there by computing numerically the vorticity in various regions of the lattice.

To ensure that we are including all possible spin configurations (and thus possible topological defects) we used two tests. First, at $\alpha_1 = 0.5$ we ran our MC starting from a more ordered configuration as well a from a more disordered configuration and found no statistically significant change in any quantity. Second, at $\alpha_1 = 0.54$ we started from a configuration with an instanton already on the lattice and found after equilibrium that the results were the same as those started from a previous MC run. Thus we believe that our MC procedure will include instantons if they are there. It would be an interesting analytic calculation to determine the effect of instantons on $\beta(K)$ and compare with our results.

D. Susceptibility

In Fig. 6 we show the susceptibility, χ, as calculated from various methods. χ cannot be calculated directly from $\beta(K)$ because of spin rescaling considerations. The high-temperature series results are from a ten-term series.[17] The Monte Carlo data begin to deviate from HT above $K = 0.90$. χ can be calculated accurately from MC only when the correlation length is a few times smaller than the size of the system. The finite size of the lattice tends to cause χ to be smaller than the true thermodynamic χ because one loses correlations which contribute to χ at large distances. One way to estimate the effect is to assume that the spin-spin correlation function $C(r)$ decays exponentially and compare the integral over $C(r)$ for an infinite system with that of a periodic lattice of length L. For example, for $L/\xi = 5$ we expect χ from the MC calculation to be about 96% of its true value.

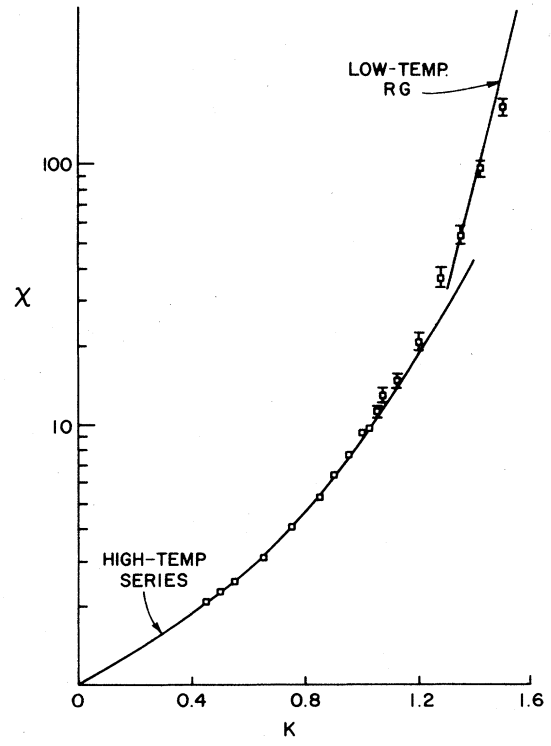

FIG. 6. Susceptibility, χ vs K. Squares are MC data calculated using one-coupling Hamiltonians. Normalization of χ is such that $\chi = 1$ for $K = 0$.

At $K = 1.42$ we estimate $\xi = 7$, thus for $L = 32$ our MC result is probably around 95% of the true value. From our MC data on χ at $K = 1.42$ we estimate that χ for an infinite lattice is about 100. (MC data give 96 ± 5.) It is important to obtain a reliable value for χ at $K = 1.42$ because the value of ΔK which takes you from some K to $K = 1.42$ agrees with the low-temperature RG results. Thus, we can determine the amplitude of the low-temperature susceptibility, which is given to two-loop accuracy by:

$$\chi = Ce^{4\pi K}\left(\frac{1}{2\pi K + 1}\right)^4 . \tag{15}$$

This form results from integrating the two-loop β function exactly and not taking the large-K limit. See Brezin and Zinn-Justin (Ref. 7). From our data we find $C = 0.018$, which is probably accurate to within 50%, although analytic corrections could very well be large.

Fisher and Nelson[18] tried to find C by matching the low- and high-temperature results for χ. They did not use $\beta(K)$ to two loops, thus changing the prefactor appearing in Eq. (15), making direct comparison difficult. However, a rough estimate indicates their method will produce a result off by a few orders of magnitude.

VI. CONCLUSION

Using the MCRG technique we have been able to map out the behavior of the three-component classical Heisenberg model. We have followed the model from deep in the low-temperature spin-wave regime, where we make quantitative contact with Polyakov's LTRG, through the crossover, all the way to the high-temperature regime, joining onto high-temperature series expansions. These results provide very strong evidence that the model has exponentially decaying correlations for all temperatures—there is no phase transition.

We can calculate the behavior of the model [such as Eqs. (14) and (15)] quantitatively, and examine the very interesting crossover regime in detail. The crossover is so sharp that 1–2 doublings of length scales are enough to take one from the low- to high-temperature regime. Aside from their intrinsic interest we hope these results can serve as benchmarks against which other approximation techniques, developed for this model or for the analogous gauge theory, can be tested.

The calculation also serves to demonstrate the utility of the MCRG technqiue. There are many methodological questions left to explore (the breakdown at high T in particular) but the simplicity and generality of the method seem to invite extensive application. Any system that can be simulated and for which a blocking rule can be defined becomes a candidate problem. We hope the method lives up to its promise.

ACKNOWLEDGMENTS

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