

# Calculation of effective Hamiltonians for renormalized or non-Hamiltonian systems

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We develop a method for calculating renormalized Hamiltonians based on the Brandt-Ron representation of renormalization-group transformations. Our approach allows us to make a stable calculation for larger sets of renormalized coupling constants than either the Swendsen or the Gupta-Cordery methods, thus reducing the effects of truncation in renormalization-group calculations. The generality of the Brandt-Ron representation also makes it suitable for analyzing a broader class of models including driven diffusive systems. Another advantage of our approach is that it contains internal criteria that provide information on the error involved in truncation approximations.

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## I. INTRODUCTION

In the renormalization-group (RG) theory of critical phenomena, the determination of critical properties is reduced to the calculation of trajectories (sequences of renormalized Hamiltonians) near a fixed point of the renormalization-group transformation. Although some methods of computation avoid the problem of directly calculating the renormalized Hamiltonians to obtain critical exponents [1], an explicit calculation is required for complete information. For Monte Carlo renormalization-group (MCRG) calculations, several methods have been created for this purpose [2]. In 1983, Swendsen [3] used a comparison between two methods of calculating correlation functions, one of which explicitly used the values of the renormalized couplings. Since they gave the same answers only when the correct renormalized couplings were used, this provided a method for determining their values. In 1984, Gupta and Cordery [4] developed a very elegant approach, which had several advantages over Swendsen's technique. Their simulation involved both the original and the renormalized spins in a novel ensemble, and all correlation functions vanished when they had found the correct renormalized couplings.

Despite the successes of these two approaches, they still have limitations on the number of couplings that can be calculated and the accuracy that can be attained. In this paper, we introduce a different approach to the problem, which allows us to compute more interactions with higher accuracy than either of the two earlier approaches.

In addition to improving the calculation of renormalized Hamiltonians within the context of renormalization-group theory, our method also allows us to investigate non-Hamiltonian dynamical systems from an unusual viewpoint. Since the static properties of non-Hamiltonian dynamical systems can be analyzed directly with our methods, we can calculate the (seemingly paradoxical) Hamiltonian representation of non-Hamiltonian systems. There is actually no contradiction or paradox involved in these statements. The static properties of any dynamical system can always, in principle, be described by a Hamiltonian. It is a separate question as to

whether that Hamiltonian has convenient properties for use in further analysis. For example, to be useful for an RG analysis, a renormalized Hamiltonian should be short-ranged. One model for which we have done calculations turns out to be short-ranged, while others are known to contain long-ranged couplings [5].

To introduce our approach, consider the Ising model of spins on a lattice that take on the values of  $+1$  and  $-1$ . The Hamiltonian for such a model is usually written in the form

$$\mathcal{H} = \sum_i K_i S_i, \quad (1)$$

where the  $S_i$ 's are various products of the spins. For example, the nearest-neighbor operator is given by

$$S_{nn} = \sum_{(j,k)} s_j s_k \quad (2)$$

and the sum runs over all nearest-neighbor pairs.

Although the Hamiltonian representation appears to be very general, it is easy to demonstrate that it is insufficient to represent all dynamical interactions. Consider a translationally invariant, two-dimensional model of Ising spins with no interactions extending beyond the nearest neighbors. Let the conditional probability distribution of any chosen spin depend only on the values of its four neighboring spins. Let the probability of the central spin taking on the value  $+1$  be given by

$$P_+^4(s_1, s_2, s_3, s_4) = \begin{cases} u_4 & \text{if } S=4 \\ u_2 & \text{if } S=2 \\ 1/2 & \text{if } S=0 \\ (1-u_2) & \text{if } S=-2 \\ (1-u_4) & \text{if } S=-4, \end{cases} \quad (3)$$

where  $S = \sum_{l=1}^4 s_l$ . In general,  $u_2$  and  $u_4$  can take on any values between 0 and 1. However, a Hamiltonian description

of this model is restricted to the nearest-neighbor sum given in Eq. (2), with a single coupling constant  $K$ . The values of  $u_2$  and  $u_4$  are then given by

$$u_n = [1 + \exp(-2nK)]^{-1}, \quad n=2,4 \quad (4)$$

and they are not free to vary independently. For given values of  $u_2$  and  $u_4$ , the model can be represented by a Hamiltonian if and only if there exists a value of  $K$  that reproduces those values through Eq. (4).

Note that a Hamiltonian representation of this dynamics cannot be saved by introducing a four-spin interaction. Although a four-spin interaction could be placed in the set of a central spin and its four neighbors, translational invariance would demand that it also be placed in other positions that would require the central spin to be influenced by spins outside this group, contradicting the assumptions of the model.

As we will show below, the Brandt-Ron representation [6] is more general than the Hamiltonian representation, and is easily able to deal with non-Hamiltonian dynamics without further approximation. This capability will be used to analyze such systems in future work.

In the course of analyzing the renormalized configurations, we are also able to test the consistency of sets of renormalized coupling constants previously generated by Swendsen and Gupta-Cordery, as well as developing a different method for calculating renormalized coupling constants from the Brandt-Ron representation.

## II. BRANDT-RON REPRESENTATION OF INTERACTIONS

The essential idea behind the Brandt-Ron representation is to describe the interactions between spins by calculating the conditional probability of given spin taking on the value of  $+1$  when the explicit values of a set of neighboring spins are specified. We shall follow the notation of Brandt and Ron and call a specific set of neighboring spins and their values a ‘‘neighborhood.’’ The conditional probability that the central spin will take on the value of  $+1$ , given the specific values of the spins in its neighborhood, is denoted by  $P_+^m(s_1, s_2, \dots, s_m)$ , where  $m$  is the number of spins in the particular neighborhood under consideration. Since the set of sites in a neighborhood will be taken to have the symmetry of the lattice,  $m$  may take on values of 4 (nearest neighbors), 8 (nearest and second-nearest neighbors), 12, 20, etc. For all the cases we consider,  $m$  will uniquely determine the set of sites in a neighborhood, while the explicit values taken on by those spins are necessary to complete the specification of a particular neighborhood. All neighborhoods that are related by an exact symmetry operation (rotation, reflection, or spin inversion) are grouped together, since those related by rotation or reflection have identical values of  $P_+^m$  and those related by spin inversion simply change  $P_+^m$  to  $1 - P_+^m$ . In the example of  $P_+^4$  given in Eq. (3), all neighborhoods with three equal spins are grouped together, as are the two neighborhoods with all spins up and all spins down.

From a Monte Carlo (MC) simulation on a given fine grid, Brandt and Ron generated a sequence of renormalized

21	20	9	13	22
19	5	1	6	14
12	4	$s_0$	2	10
18	8	3	7	15
24	17	11	16	23

FIG. 1. The 24-spin neighborhood surrounding a spin  $s_0$ .

(block spin) configurations, using the majority-rule transformation on  $2 \times 2$  blocks, although the method can be used equally well with any other RG transformation. For every spin in every generated renormalized configuration, the surrounding neighborhood was identified and the accumulated number of its total occurrences and that for which the central spin was  $+1$  were updated. The desired  $P_+^m$  values easily follow.

The  $P_+$  table provides a very general representation of the interactions. For example, there are a total of 314 distinct neighborhoods on the nearest 12 sites shown in Fig. 1. However, there are only five terms in the most general Hamiltonian that can be defined within the limits of these 12 sites.

In the rest of the paper, most of the calculations will refer to the sites in a 20-spin neighborhood shown in Fig. 1. Brandt and Ron used a total of 80 384 neighborhoods in their analysis of the renormalized interactions of the two-dimensional Ising model simulated at the critical point where  $K=0.440\,686\,8$ . This large number of neighborhoods comes from the 314 12-spin neighborhoods, multiplied by the  $2^8$  different arrangement of spin values on the additional eight sites. For simplicity in programming, no symmetries were used for the additional eight sites to reduce the total number of neighborhoods, which are not all distinct.

Naturally, different neighborhoods occur with differing probabilities. Table I lists a great deal of information for the 12 most common neighborhoods, which together account for over 50% of the observations at the critical point. The column labeled ‘‘ $w$ ’’ gives the relative frequency of each neighborhood. These neighborhoods are all composed of mostly positive spins. The left column identifies which spins out of the 20-spin neighborhood shown in Fig. 1 take on the value  $-1$ . Observe that none of the neighborhoods has more than two spins out of 20 with the value  $-1$  and that the most common neighborhood contains only positive spins, and occurs in nearly one-quarter of the measurements.

Since the specification of a neighborhood begins with the choice of a finite set of spins, a truncation of the full set of renormalized interactions is inevitable. If the error caused by this truncation falls off rapidly as the set of spins used for the neighborhoods is increased, the model is said to possess ‘‘near locality’’ in the terminology of Brandt and Ron. In their work, Brandt and Ron used a sophisticated algorithm that constructed an appropriate set of growing neighborhoods for a given degree of accuracy during the course of a Monte Carlo simulation [6]. We will use their results for the set of

TABLE I. The  $P_+$ 's of the first renormalized level obtained by Gupta-Cordery (GC) and by Brandt-Ron (BR) for the 20-spin neighborhood shown in Fig. 1.

Neighborhood - 1 at:	First renormalized level				
	GC	BR	BR-12	BR-21	$w$
	0.97096(38)	0.970456(1)	0.970380(31)	0.970425(80)	0.2374
13	0.97094(34)	0.970420(2)	0.970362(27)	0.970395(66)	0.1044
9	0.97046(33)	0.970332(3)	0.970240(26)	0.970275(61)	0.0400
1	0.87045(88)	0.868889(6)	0.869444(68)	0.868790(132)	0.0323
5	0.95839(34)	0.956307(1)	0.957087(27)	0.956496(63)	0.0301
6,13	0.95954(31)	0.958618(6)	0.958835(24)	0.958737(60)	0.0168
1,5	0.83144(74)	0.829299(14)	0.828858(55)	0.828954(135)	0.0104
9,13	0.97054(29)	0.970299(5)	0.970255(24)	0.970310(58)	0.0104
9,14	0.97053(29)	0.970301(7)	0.970320(23)	0.970281(51)	0.0104
9,15	0.97044(28)	0.970299(6)	0.970222(22)	0.970245(47)	0.0104
9,16	0.97044(28)	0.970306(2)	0.970222(22)	0.970245(47)	0.0104
13,14	0.97109(31)	0.970625(3)	0.970493(26)	0.970647(60)	0.0083

20-spin neighborhoods and the values of the 80 384  $P_+$ 's that they measured.

Because Brandt and Ron provided data that demonstrate near locality for these neighborhoods, we know that truncation to 20-spin neighborhoods introduces a very small error. For example, consider the  $P_+$ 's for a sequence of neighborhoods of increasing size with all spins having the value +1. The values are

$$P_+^4 = 0.967\,040$$

$$P_+^8 = 0.970\,422, \quad P_+^8 - P_+^4 = 0.003\,382;$$

$$P_+^{12} = 0.970\,446, \quad P_+^{12} - P_+^8 = 0.000\,024;$$

$$P_+^{20} = 0.970\,456, \quad P_+^{20} - P_+^{12} = 0.000\,010;$$

$$P_+^{24} = 0.970\,460, \quad P_+^{24} - P_+^{20} = 0.000\,004.$$

The changes in  $P_+^m$  rapidly become smaller as  $m$  is increased, with the difference between a 12-spin neighborhood and a 20-spin neighborhood being only one part in  $10^5$ . This is consistent with the assumption of near locality, and justifies the assumption that 20-spin neighborhoods are sufficient for the purposes of this paper.

### III. COMPARISON OF MEASURED $P_+$ 'S WITH MCRG CALCULATIONS

The data we will use for the  $P_+$ 's are taken from the work of Brandt and Ron. The particular results were generated using three Wolff [7] cluster updates between each measurement of data from a configuration for  $5 \times 10^7$  measurements on a  $128 \times 128$  lattice. Three cluster flips were chosen because that corresponds roughly to flipping every spin in the lattice once on average. It should be noted that the  $P_+$ 's are local quantities that do not depend on the establishment of global equilibrium, which makes them particularly easy to calculate to high accuracy. Any critical slowing down due to

the algorithm used will affect the determination of the frequencies of observing each neighborhood,  $w_j$ , rather than the  $P_+$ 's.

Given a model with a Hamiltonian representation described by Eq. (1), the  $P_+$ 's can be calculated directly from the values of the coupling constants using the equation

$$P_+ = [1 + \exp(-2\mathcal{H}(s))]^{-1}, \quad (5)$$

where  $s$  is the set of spins that take on the values specified by the neighborhood.

In Tables I and II, we begin our comparison with the Gupta-Cordery results. The neighborhoods are associated with the 20-spin neighborhood shown in Fig. 1. For each neighborhood, all spins are positive except for the spins at the specified locations, which are negative. The columns labeled "GC" were generated from 12 out of the 14 Gupta-Cordery coupling constants, using Eq. (5). We neglected the two Gupta-Cordery coupling constants that fell outside the range of our 20-spin neighborhoods. The columns labeled "BR" were taken from the Brandt-Ron results.

Looking at the columns for the first renormalized level in Table I, the similarity of the results from the Gupta-Cordery and Brandt-Ron calculations is immediately apparent. However, there is also a striking systematic difference between the results in that every  $P_+$  generated from the Gupta-Cordery couplings are systematically higher than those measured by Brandt and Ron. We conclude that Gupta and Cordery succeeded in doing an excellent calculation of the effective renormalized couplings within their truncation, but the overall strength of those couplings is systematically too high, at least when the additional two couplings are neglected. These values for the renormalized couplings correspond to a model that is slightly off-critical hypersurface, with too low an effective temperature. To test the possible effect of adding the two extra couplings specified by Gupta and Cordery, we have calculated the  $P_+$  for a 24-spin neighborhood of all spins taking the value +1 and obtained 0.971 956. The corresponding Brandt-Ron result is

TABLE II. The  $P_+$ 's of the second renormalized level obtained by Gupta-Cordery (GC) and by Brandt-Ron (BR) for the 20-spin neighborhood shown in Fig. 1.

Neighborhood - 1 at:	Second renormalized level			
	GC	BR	BR-12	$w$
	0.97199(86)	0.969912(2)	0.969902(59)	0.2417
13	0.97187(76)	0.969888(6)	0.969870(52)	0.1060
9	0.97146(73)	0.969893(3)	0.969821(49)	0.0412
1	0.87806(186)	0.873739(5)	0.874432(122)	0.0333
5	0.95757(78)	0.953144(1)	0.954183(52)	0.0315
6,13	0.95929(71)	0.955914(7)	0.956248(49)	0.0166
1,5	0.83041(166)	0.824308(5)	0.824751(102)	0.0105
9,13	0.97153(65)	0.969901(6)	0.969872(44)	0.0103
9,14	0.97150(64)	0.969904(3)	0.969919(43)	0.0103
9,15	0.97135(63)	0.969902(7)	0.969789(42)	0.0103
9,16	0.97135(63)	0.969904(5)	0.969789(42)	0.0103
13,14	0.97189(69)	0.970073(9)	0.969920(48)	0.0085

0.970460, showing an even larger discrepancy. A similar deviation was observed also for the 24-spin neighborhood of all spins +1 except one negative spin at site 13: Gupta and Cordery predicted 0.971733 while Brandt-Ron measured 0.970390.

The columns in Table II for the second renormalized level are consistent with this interpretation. Again the Gupta-Cordery  $P_+$ 's are quite close to the Brandt-Ron values, but are systematically too high. Since the deviation from criticality corresponds to a relevant direction, the deviations in the second renormalized level are expected to be larger, which is observed to be the case. The larger statistical errors are due to the smaller grid size obtained after two RG transformations.

Apart from the small deviations of the Gupta-Cordery couplings from criticality, the good agreement with the Brandt-Ron results demonstrates an encouraging consistency. However, for a more complete comparison, we need to calculate the renormalized coupling constants from the measured  $P_+$ 's. This will be done in the following sections.

#### IV. CALCULATION OF COUPLINGS FROM $P_+$ 'S

In order to invert Eq. (5) to calculate the renormalized couplings from the  $P_+$ 's, we need to deal with the fact that there are many more  $P_+$ 's than there are renormalized couplings. Our procedure will be to determine renormalized couplings by minimizing the sum of the weighted deviations of the  $P_+$ 's calculated from Eq. (5) from those measured by Brandt and Ron.

For convenience, instead of using the  $P_+$ 's directly, we define a cost function in terms of the quantities

$$\mathcal{H}_j = -(1/2)\ln[(1 - P_j)/P_j], \quad (6)$$

where the index  $j$  refers to the  $j$ th entry in the corresponding  $P_+$  table. This choice simplifies the minimization process to merely solving a linear system of equations. Our cost function is then given by

$$\mathcal{F} = \frac{1}{4M} \sum_j \left( \mathcal{H}_j - \sum_i K_i S_{ij} \right)^2 / [\delta\mathcal{H}_j]^2, \quad (7)$$

where the  $K_i$ 's are the desired coupling constants, the  $S_{ij}$ 's are the various products of spins evaluated for the  $j$ th neighborhood, and  $\delta\mathcal{H}_j$  is the standard deviation of  $\mathcal{H}_j$ , which is related to the standard deviation of  $P_j$  through the equation

$$\delta\mathcal{H}_j = (1/2)[P_j(1 - P_j)]^{-1} \delta P_j. \quad (8)$$

Since  $P_j$  is calculated by averaging the values of the central spin for each neighborhood, its error is governed by the binomial distribution, so that

$$(\delta P_j)^2 = P_j(1 - P_j)/M_j, \quad (9)$$

where  $M_j$  is the total number of instances of neighborhood  $j$  observed during the simulation. Since we have one neighborhood surrounding every spin in every configuration, the total number of occurrences of all neighborhoods is

$$M = \sum_j M_j = CL^2, \quad (10)$$

where  $C$  is the total number of configurations and  $L^2$  is the number of spins (and neighborhoods) in each configuration. Expressing this in terms of the relative frequency of each neighborhood,  $w_j = M_j/M$ , we arrive at the following expression for the cost function:

$$\mathcal{F} = \sum_j \left( \mathcal{H}_j - \sum_i K_i S_{ij} \right)^2 w_j P_j (1 - P_j). \quad (11)$$

#### V. COMPARISON OF CALCULATED RENORMALIZED COUPLINGS WITH MCRG CALCULATIONS

All methods for calculating renormalized couplings necessarily involve some sort of truncation. To investigate the effective truncation, we begin the comparison with the early calculation by Swendsen involving a rather severe truncation

TABLE III. The 6-coupling constants calculated by Swendsen and by Brandt-Ron (BR) for the first renormalized level.

Type of interaction	First renormalized level	
	Swendsen (32 <sup>2</sup> )	BR (128 <sup>2</sup> )
012		
345		
678		
01	0.3643(6)	0.363457(9)
04	0.0814(8)	0.081449(7)
02	-0.0068(2)	-0.007091(6)
05	-0.0038(3)	-0.004396(3)
0134	-0.0077(6)	-0.008825(7)
1357	0.0026(5)	0.002650(4)

to only 6-coupling constants. Table III gives both Swendsen's values for the couplings and our results for the same truncation found by minimizing the cost function (11) described in the preceding section. The overall agreement is quite good, although the new results are much more accurate. In all cases, the differences are within one or two standard deviations of the original calculation.

Table IV shows a similar comparison with a more extended set of 12-coupling constants calculated by Gupta and Cordery. In addition to using more couplings than Swendsen in their analysis, Gupta and Cordery also introduced an improved method that produced smaller errors.

Actually, Gupta and Cordery used a set of 14 couplings in their calculations, but we have only taken 12 into account in our comparison because the additional two couplings were outside our largest neighborhoods. Although there is good overall agreement between our results and those of Gupta and Cordery, there are also significant differences that are

much larger than the statistical errors of each calculation. For example, the nearest-neighbor coupling with a 6-coupling truncation has the value 0.363 457(9), while the 12-coupling truncation gives the lower value of 0.351 436(8). The Gupta-Cordery result from a 14-coupling truncation gives a value that is shifted to 0.353 58(10), even though the values of the additional couplings were smaller than this shift. This pattern of general agreement but with deviations that greatly exceed the statistical errors of each calculation is repeated for all the couplings in the table. The most extreme deviation is that for the 1357 four-spin interaction, for which the sign of the coupling constant changes between the 6-coupling truncation and either the 12-coupling (this work) or 14-coupling (GC) truncations.

An advantage of our approach for calculating renormalized coupling constants is that we are able to find stable results for larger sets of couplings than with either the Swendsen or the Gupta-Cordery approaches. This enabled us to extend the investigation of the effects of truncation to perform a calculation with 21 couplings, as shown in Table V. These 21 couplings represent the complete set of couplings that are consistent with the 20-site neighborhood shown in Fig. 1. There is again good general agreement with the 12-coupling truncation, but significant shifts in the individual values. The nearest-neighbor coupling constant is now 0.353 112(14), which differs from the 12-coupling truncation result in the third digit, even though the added couplings are of much longer range and very weak. Our general conclusion is that truncated approximations are very sensitive to the number of operators used, even when the neglected operators have very small coupling constants associated with them. This casts some doubt on the ultimate reliability of any determination of a set of renormalized couplings. The general picture of the renormalized couplings is probably correct, but the explicit values calculated are probably not nearly as accurate as the statistical error might lead one to believe.

TABLE IV. The 12-coupling constants calculated by Gupta-Cordery (GC) and by Brandt-Ron (BR) for the first and the second renormalized levels.

Type of interaction	First renormalized level		Second renormalized level	
	GC (128 <sup>2</sup> )	BR (128 <sup>2</sup> )	GC (128 <sup>2</sup> )	BR (128 <sup>2</sup> )
012				
345				
678				
01	0.35358(10)	0.351436(8)	0.34608(24)	0.340138(20)
04	0.07488(10)	0.076717(5)	0.08845(23)	0.089627(18)
02	-0.00758(9)	-0.008779(11)	-0.00929(22)	-0.010948(9)
05	-0.00618(7)	-0.006560(5)	-0.00700(14)	-0.007155(5)
0134	-0.01522(9)	-0.014245(8)	-0.01895(21)	-0.017328(9)
1345	0.00760(4)	0.006493(3)	0.00733(10)	0.006018(7)
1357	-0.00582(7)	-0.004410(4)	-0.00524(17)	-0.003119(16)
0457	0.00289(4)	0.003399(4)	0.00286(9)	0.003186(5)
0123	0.00152(3)	0.001520(3)	0.00194(7)	0.001731(3)
0145	0.00101(4)	0.001537(4)	0.00156(10)	0.002041(7)
0157	-0.00107(3)	-0.001377(2)	-0.00112(6)	-0.001422(6)
0247	0.00040(4)	0.000424(4)	0.00068(9)	0.000580(5)

TABLE V. The complete set of 21-coupling constants calculated by Brandt-Ron (BR) for the first renormalized level.

Type of interaction	First renormalized level	Type of interaction	First renormalized level (cont.)
012	BR	012	BR
345	(128 <sup>2</sup> )	345	(128 <sup>2</sup> )
678		678	
01	0.353112(14)	0247	0.000679(4)
04	0.076058(12)	0127	-0.000580(5)
02	-0.008700(13)	0167	-0.000493(4)
05	-0.005993(6)	0135	0.000138(6)
0134	-0.015290(18)	0156	-0.000317(2)
1345	0.006555(5)	012345	0.000185(4)
1357	-0.004809(4)	013457	0.000050(3)
0457	0.003096(5)	012347	0.000293(2)
0123	0.001338(4)	012357	-0.000088(3)
0145	0.000992(4)	014567	0.000191(3)
0157	-0.001034(2)		

## VI. INTERNAL CONSISTENCY OF RESULTS

Keeping in mind that any truncation inevitably introduces some systematic error that would produce discrepancies between the predictions of the approximate Hamiltonian and the measured values of the  $P_+$ 's, we have looked at the systematic changes in  $\mathcal{F}$ , the cost function defined in Sec. IV, Eq. (11).

Using only the 6-coupling constants shown in Table III as determined by our method, we find that the value of  $\mathcal{F}$  is 0.000 16, so that discrepancies between the data and the predictions of this truncated Hamiltonian are clearly measurable. Even so, the deviations from the measured values of the  $P_+$ 's lie in the fourth significant digit.

When we improve the truncation by using the 12 couplings determined by our method, which are shown in Table IV, we find that the value of  $\mathcal{F}$  is only 0.000 002 8. Furthermore, when we use the 21-coupling set shown in Table V, the value of  $\mathcal{F}$  is reduced to 0.000 002 3.

We have also investigated the second level of renormalization with the couplings shown in Table IV. The value of  $\mathcal{F}$  for these 12 couplings is 0.000 003 4, which is close to the value of 0.000 002 8 for the same truncation in the first level of renormalization, as expected.

As another test of consistency, we investigated a sequence of growing neighborhoods to analyze a  $1 \times 10^6$  configuration simulation of a  $128^2$  lattice. Table VI shows the effect on the cost function when the size of the neighborhood is increased. Although the first row of the table corresponds to an extreme truncation, the cost function turns out to be artificially low because there are only two  $P_+$ 's to be fit by the single coupling. As the neighborhoods grow, the number of  $P_+$ 's increases much more rapidly than the number of couplings in the effective Hamiltonian. For the eight-spin neighborhood, the effect of having to fit more parameters dominates, but as the neighborhoods become larger, the great improvement of the truncation approximation is the determining factor that drives the value of the cost function down rapidly.

TABLE VI. The cost function  $\mathcal{F}$  calculated for  $m$ -spin neighborhoods ( $m=4,8,12,20$ ) for the first renormalized level.

$m$	Number of neighborhoods	Number of coupling constants	$\mathcal{F}$
4	2	1	0.000021
8	24	3	0.000132
12	304	5	0.000018
20	80384 <sup>a</sup>	21	0.0000023

<sup>a</sup>Not all distinct.

Another way of checking on the consistency of our results is simply to compare the individual  $P_+$ 's with the predictions of our calculated couplings. In Tables I and II, we have shown such a comparison for the leading 12  $P_+$ 's, which represent over 50% of the observations of a neighborhood. The columns marked ‘‘BR-12’’ contain the predictions for the  $P_+$ 's from the sets of 12-coupling constants for both the first and second levels of renormalization. Discrepancies can be clearly seen between the measured and predicted values. However, comparison with the Gupta-Cordery results presented in the same table shows that there has been substantial improvement. A further improvement is seen for the first renormalized system by calculating the  $P_+$ 's from the 21-coupling constants, the column marked ‘‘BR-21.’’ Again, since the differences are quite small, we conclude that our calculated couplings provide a good approximation for the Hamiltonian.

## VII. DYNAMICAL SYSTEMS

To present our results for dynamical systems, it will be useful to consider a specific example in some detail. We have performed extensive simulations of non-Hamiltonian dynamics on a  $3 \times 3$  lattice with periodic boundary conditions. We used the nearest-neighbor dynamics introduced in Eq. (3), with  $u_2 = u_4 = 0.9$ , which cannot be represented by a nearest-neighbor Hamiltonian. Because the system is so small, we were able to make a very long run of  $10^8$  MC sweeps to calculate the  $P_+^8$  table for the eight-spin neighborhood in the steady state.

As a first consistency check, we then did a new simulation on the same lattice using this  $P_+^8$  table. Naturally, this new simulation satisfies detailed balance, although the original simulation did not. The  $P_+^8$  table measured from the new simulation was identical to the original one within the small statistical errors.

Next, we used the method described above to calculate the 12-coupling constants that fit on a  $3 \times 3$  lattice from the measured  $P_+^8$  table. Because this is a complete set with no truncation, the cost function was zero to within the numerical accuracy of the calculation. As a further check on these results, we also solved an overdetermined set of linear equations for the couplings and found a solution that matched the one obtained by minimizing the cost function.

This immediately demonstrates that we can have two different dynamics that lead to the same steady state, even though one is clearly non-Hamiltonian and the other is based

TABLE VII. The 5-coupling constants calculated from  $P_+^{12}$  (on a  $64 \times 64$  lattice) and the corresponding values of the cost function  $\mathcal{F}$  for three different dynamics.

Type of interaction	$u_2=11/12$ and $u_4=0.9$	First renormalized level	$K=0.45$ or $K=0$
012	MC	RG	MC
345	( $64^2$ )	( $128^2$ )	( $64^2$ )
678			
01	0.36332	0.35623	0.15732
04	0.05797	0.05658	0.00106
02	0.02708	-0.01371	0.00055
0134	-0.00535	-0.01191	-0.00015
1345	-0.03613	0.00971	-0.00169
$\mathcal{F}$	0.000576	0.000018	0.0000077

on a Hamiltonian. This shows that the distinction between Hamiltonian and non-Hamiltonian systems lies completely in the dynamics, and is not reflected in some property of the statics.

From a simulation of dynamics that clearly depends only on nearest neighbors, but is not describable by a nearest-neighbor Hamiltonian, we obtained an equilibrium distribution that is described by a longer-range Hamiltonian.

We have confirmed these observations with more general tests. On a  $64^2$  lattice, we have used the nearest-neighbor, non-Hamiltonian dynamics with  $u_2=11/12$  and  $u_4=0.9$ . These values were chosen because the effective Hamiltonian for the 12-spin neighborhood is close to that obtained from the renormalization of a nearest-neighbor Ising model at criticality. We also looked at a two-temperature model, for which the coupling constant for each update was randomly chosen to be either  $K=0.45$  or  $K=0$ . The values obtained for the five couplings that fit in this neighborhood, along with the corresponding values of the cost function, are shown in Table VII for all of these models.

It can be seen from this table that, although the couplings for the  $u_2-u_4$  model fall off with distance, they are still larger than those for the renormalized Hamiltonian. This pattern is supported by the values of the cost function, which is larger for the  $u_2-u_4$  model. This gives us the somewhat surprising result that a model with explicitly nearest-neighbor dynamical interactions corresponds to a longer-range Hamiltonian than a renormalized Ising model.

By contrast, the two-temperature model corresponds to a nearly nearest-neighbor Hamiltonian with a very small value for the cost function, indicating that the more distant cou-

plings are also very small. This is consistent with the known result that this model is in the same universality class as the Ising model.

In summary, we have shown by explicit example how the steady-state distribution for a nearest-neighbor non-Hamiltonian dynamics is indistinguishable from an equilibrium distribution for a longer-range Hamiltonian. It is naturally an interesting question to ask whether we can find a short-range non-Hamiltonian dynamics for a longer-range Hamiltonian, such as the renormalized Ising Hamiltonian. A count of the number of parameters available for each description suggests that this is feasible. It would also be interesting to know if a nearest-neighbor Hamiltonian can be represented by a longer- but still finite-ranged non-Hamiltonian dynamics. Our results suggest that this is also possible, but no example has yet been constructed.

## VIII. CONCLUSIONS

We have shown how the Brandt-Ron representation can be used to calculate consistent sets of renormalized coupling constants. Furthermore, since the Brandt-Ron representation is very general, it can be used to determine whether coupling constants calculated with any method are consistent with the data obtained for a large set of neighborhoods. For the case considered, the two-dimensional Ising model with a  $2 \times 2$  majority-rule renormalization-group transformation, we found that good approximations could be obtained with reasonably small truncation errors.

On the other hand, we also showed that truncations can have a much larger effect than is usually assumed. Adding couplings can produce significant changes in all other couplings, even when the new couplings have very small amplitudes.

We have also shown that the distinction between Hamiltonian and non-Hamiltonian systems lies entirely in the dynamics. There is no essential difference in the static distribution between steady state and thermal equilibrium.

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