DETERMINATION OF CRITICAL POINTS AND FLOW DIAGRAMS BY MONTE CARLO RENORMALIZATION GROUP METHODS

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A general method for calculating block renormalized coupling constants within the framework of the Monte Carlo renormalization group is presented. The method is applicable for any values of the couplings and in particular for those far from the critical point. A new technique for evaluating separately the derivatives of the block renormalized couplings is also discussed. The utility of these methods is demonstrated on the two-dimensional Ising model, where knowledge of the exact critical point in the multiparameter space of coupling constants results in improved values of the critical exponents.

1. Prolegomena

The Monte Carlo renormalization group is known to give accurate and reliable information about the critical properties of statistical systems [1–4] [‡1] and lattice gauge theories [5,6]. It is a combination of the principles of Monte Carlo simulation [7] with those of the real-space renormalization group [8]. The system under consideration is divided into "blocks", and a smaller number of block variables are defined by averaging in some fashion over the original "site" variables. By studying the way in which the site hamiltonian (or lagrangian for lattice gauge theories) "flows" into the block renormalized hamiltonian the critical properties of the system can be determined.

One difficulty of the Monte Carlo renormalization group procedure is that while it is known [2] how to obtain the derivatives of the renormalized couplings with respect to the original couplings, previously no general method for determining the couplings themselves has been presented. A popular method originally proposed by Wilson [5] works only in the neighborhood of the fixed point.

Here we present a procedure which can be used to calculate the block renormalized couplings (and hence the renormalization group trajectory) even far from the critical point. An advantage of this technique is that it allows one to determine all critical points and flows in the general parameter space without any a priori knowledge of the critical properties of the system. A more practical advantage is obvious: by performing the simulations at the actual critical point in the general space of interactions (rather than in the usual projected space) the accuracy of the critical exponents can be improved. The method is presented below in detail.

2. General description of the procedure

Consider a system of site variables $\{\phi\}$ governed by a site hamiltonian $H\{\phi\}$. A "renormalized" or block hamiltonian $H'\{\phi'\}$ is determined from the site hamiltonian by the use of an appropriate projection operator $P[\{\phi\}, \{\phi'\}]$,

$$e^{-H'\{\phi'\}} = \mathrm{Tr}_{\{\phi\}} P[\{\phi'\}, \{\phi\}]\, e^{-H\{\phi\}}, \tag{1}$$

where the trace (or functional integral) is only over the site variables $\{\phi\}$. The requirement that the renormalization group transformation preserve the partition function of the system imposes the constraint

$$\mathrm{Tr}_{\{\phi'\}} P[\{\phi'\}, \{\phi\}] = 1. \tag{2}$$

The projection operator is otherwise arbitrary.

For the sake of simplicity the projection operator

[‡1] The Monte Carlo renormalization group is reviewed in ref. [4].

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is usually taken to be a product of delta functions,

$$P[\{\phi'\},\{\phi\}] = \prod_i \delta[\phi'_i - g_i\{\phi\}], \quad (3)$$

where the $g_i\{\phi\}$ are some appropriately chosen functions of the $\{\phi\}$. However we find it very advantageous to use instead a "smeared" projection operator,

$$P[\{\phi'\},\{\phi\}] = N(\beta) \prod_i \exp[-\beta(\phi'_i - g_i\{\phi\})^2], \quad (4)$$

where $N(\beta)$ is a normalization factor which depends only on β. With the use of the projection operator of eq. (4) it is easy to do a simulation while holding some of the $\{\phi'\}$ fixed. It is more difficult to fix some of the $\{\phi'\}$ when the projection operator of eq. (3) is used instead because of the problems associated with inverting a delta function. For sufficiently large β, the two projection operators are of course equivalent.

It is worth emphasizing the utility of the choice eq. (4). The advantage of this "smeared" projection operator is that it allows each of the variables $\{\phi'\}$ separately either to be generated [by first producing a configuration $\{\phi\}$ and then generating one or more of the $\{\phi'\}$ using eq. (4)] or to be fixed beforehand [in which case the appropriate term(s) in the exponential eq. (4) are treated as part of the site hamiltonian $H\{\phi\}$ when the $\{\phi\}$ are generated]. Some of the block variables can be fixed in this fashion while others are allowed to fluctuate.

With the above description in mind, our prescription for calculating the block renormalized couplings is straightforward. First all of the block variables $\{\phi'\}$ but one (denoted by ϕ'_0) are fixed in a fashion prescribed below. The remaining variable is allowed to fluctuate with a distribution given by eq. (4).

Both the site and block hamiltonians can be expanded in terms of appropriate basis functions $\{S\}$ and coupling constants $\{K\}$ and $\{K'\}$ respectively as follows:

$$H'\{\phi'\} = \sum_\alpha K'_\alpha S_\alpha\{\phi'\}, \quad H\{\phi\} = \sum_\alpha K_\alpha S_\alpha\{\phi\}. \quad (5a,b)$$

The $\{\phi'_i, i \neq 0\}$ are fixed in such a fashion that all but a small number of the $\{S\}$ (e.g. one, denoted by S_0) which involve ϕ'_0 are zero in the block system. Then the probability that the lone fluctuating variable assumes the value ϕ'_0 is proportional to

$$\rho(\phi'_0) \propto \exp[K'_0 S_0\{\phi'\}], \quad (6)$$

which depends only on the chosen coupling K'_0 and the known function $S_0\{\phi'\}$. It is thus a trivial matter to determine K'_0 by measuring the function $\rho(\phi'_0)$. In this fashion all of the couplings of the theory can be evaluated systematically.

It is of course not always possible to choose a single block configuration in which all of the $\{S\}$ but the chosen one are zero. However, by suitable combinations of the results from several block configurations it is possible to separate the couplings. Additionally in practice only a small number of couplings are large, and it is often possible to separate these with a single block configuration. A specific example of this method is described below.

3. Application to the two-dimensional Ising model

3.1. Method. The formalism described in the preceding section is now applied to the two-dimensional Ising model. In this case the spin variables $\{\sigma\}$ and $\{\sigma'\}$ only take on the values ± 1. Thus the only interactions present are those between a spin and one or more of its neighbors (whether near or far); self-interactions are absent. A point of notation is in order: In fig. 1a

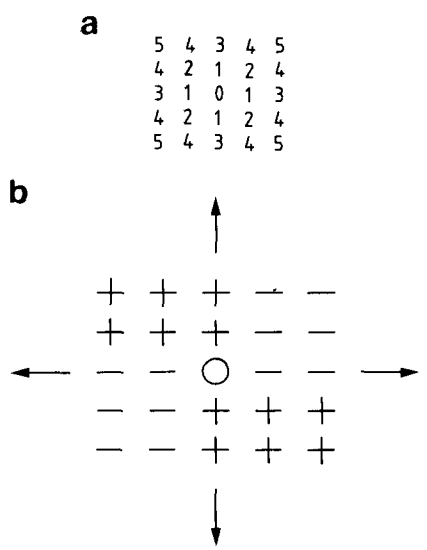

Fig. 1. (a) Schematic diagram at a spin (at 0) and its first through fifth neighbours; (b) Schematic diagram showing basic block spin configuration for cancelling even-spin interactions.

the first (or "nearest") neighbors, second neighbors, etc. of the spin at point 0 are shown. The $\{S\}$ of eqs. (5) are taken to be the sum of the interactions between the spin at point 0 and each of the classes of neighbors (including of course interactions with up to the total number of nth neighbor spins). In particular we adopt the notation that K_1 and K_2 are respectively the nearest neighbor and second neighbor two-spin couplings, while K_3 is the four-spin coupling consisting of a symmetric sum of products of a spin and three of its four nearest neighbors.

The projection operator eq. (4) for the Ising model can be written in the form,

$$P[\{\sigma'\}, \{\sigma\}] = \prod_i \exp[\beta\sigma'_i g_i\{\sigma\}]/2\cosh\beta. \qquad (7)$$

In the calculations described below, the function $g_i\{\sigma\}$ is determined by the so-called "majority rule", that is, g_i equals plus or minus one if the sum of the spins in a block is positive or negative respectively. For this calculation the lattice is divided into standard square blocks with three site spins on a side. The value $\beta = 10$ was chosen, however, using larger values of β did not make a significant difference in the results.

The method of calculation for the block renormalized couplings is as follows. One block spin (depicted as 0 in fig. 1b) is generated with a relative probability $\exp[\beta\sigma'_0 g_0\{\sigma\}]$. The rest of the block spins are fixed in such a fashion as to cancel as many of the interactions as possible, leaving only the ones of interest.

This separation is easy to perform. For simplicity, consider first the case in which the site hamiltonian has only interactions involving an even number of spins. Thus the block hamiltonian also only contains even interactions. If the block spins surrounding the fluctuating block spin σ'_0 are chosen in the fashion depicted in fig. 1b except for the four nearest neighbor spins (numbered 1 in fig. 1a), then K'_1 and K'_2 can be determined. The four nearest neighbor spins are first all set equal to one, and the number $N_+(++++)$ $[N_-(++++)]$ of times that the block spin σ'_0 takes on the value +1 [−1] is recorded. The other block spins (the "background") are fixed in the pattern fig. 1b. The above procedure is repeated for the case in which three of the four nearest neighbors are set to +1, while the fourth is set to −1. In this fashion $N_+(+++-)$ and $N_-(+++-)$ are calculated. The couplings K'_1 and K'_2 are then determined by solving the equations,

$$N_+(++++)/N_-(++++) = \exp(8K'_1 + 8K'_3),$$

$$N_+(+++-)/N_-(+++-) = \exp(4K'_1 - 4K'_3). \qquad (8)$$

In practice we found that K_3 is negligible (i.e. $K_3 < 0.01$) and so it was dropped from the calculations.

Corrections to eqs. (8) arise from the fact that the background pattern of fig. 1b actually does not cancel all other interactions, although it certainly does cancel an enormous fraction of them. For example, a four-spin interaction involving one nearest neighbor and two diagonally opposite second-neighbors is not cancelled by this prescription. This coupling is not particularly large in the case under consideration. If it was large, it would be a fairly simple matter to include three interactions in eqs. (8) and thus separate the effects of this new coupling. It is in fact a normal assumption of the renormalization-group formalism that only a small number of operators need to be considered in a calculation (provided that a sensible projection operator is used).

In a similar fashion the second neighbor coupling K'_2 is determined. The block spins are arranged in the pattern fig. 1b except for the four second neighbor spins (numbered 2 in fig. 1a). The number of times N_+ $[N_-]$ that the spin σ'_0 assumes the value +1 [−1] is again recorded and K'_2 is given by

$$K'_2 = \tfrac{1}{8}\ln[N_+/N_-]. \qquad (9)$$

A more accurate determination of the coupling K'_2 can be made by arranging the nearest neighbors in a pattern (++−−) rather than the (+−+−) pattern of fig. 1b. This latter configuration eliminates a four-spin coupling involving two nearest neighbors and one second neighbor. For our calculation this second configuration was used, although the additional accuracy proved irrelevant.

In order to determine the critical exponents of a theory the derivatives of the coupling constants are evaluated at a fixed point. These derivatives can be evaluated using the standard method [2] (discussed below) or by a method analogous to the one used above for finding the block renormalized constants. The second method allows the derivatives of the couplings to be evaluated at the same time as the renormalized couplings themselves. This new technique is presented immediately below.

Consider for example the calculation of the deriva-

tives of the block second nearest neighbor coupling K_2' with respect to the site couplings $\{K\}$. The block spins are set to the values of fig. 1b, except for the four nearest neighbor spins, which are set to one. Then (since the derivatives of the four-spin coupling are negligible) it follows by differentiating eq. (1) that

$$\frac{\partial K_2'}{\partial K_a} = \tfrac{1}{8}[\langle S_a\rangle_+ - \langle S_a\rangle_-], \tag{10}$$

where $\langle S_a\rangle_+$ $[\langle S_a\rangle_-]$ is the expectation value of the component a of the hamiltonian, with the average taken only over those configurations where the spin σ_0' equals +1 $[-1]$. With this example in mind it is easy to develop the formulae for the derivatives of the other couplings. Note that by adding and subtracting formulae like eq. (10) each derivative can be separately calculated.

For completeness the standard method [2] of calculating the derivatives of coupling constants is discussed. These derivatives are determined by measuring the expectation values,

$$C_{ab} = \langle [S_a - \langle S_a\rangle]\,[S_b - \langle S_b\rangle]\rangle \tag{11a}$$

and

$$C'_{ab} = \langle [S'_a - \langle S'_a\rangle]\,[S_b - \langle S_b\rangle]\rangle. \tag{11b}$$

In practice, only a small number of the elements of the matrices C and C' are measured, i.e., a and b range from one to some number N_{corr}.

The derivatives of the block renormalized couplings are determined by the solution of the matrix equation,

$$C = DC', \tag{12a}$$

where

$$D_{ab} = \partial K'_a/\partial K_b. \tag{12b}$$

The critical eigenvalues are then determined by the diagonalization of the matrix D, using only the first $(N_{\mathrm{eigen}})^2$ elements.

In our review of this latter technique, we have made explicit the difference between the number of correlations measured, N_{corr}, and the number of elements, N_{eigen}, used in the diagonalization. The point is the following. With our procedure for calculating derivatives [as defined in eq. (9)] it is possible in principle to evaluate separately a number of derivatives without calculating the derivative of every block renormalized coupling with respect to every site coupling. In the standard method [2], this luxury is note permitted – in order to find the matrix D in principle all of the elements of the matrices C and C' must be known.

In practice what we have done to compare the two methods is to increase the number N_{corr} of measured correlations until the first $(N_{\mathrm{eigen}})^2$ elements of D are stable against the inclusion of additional interactions. The eigenvalues of this stable submatrix are then computed. This procedure provides the fairest comparison between the two methods if the $N_{\mathrm{corr}} - N_{\mathrm{eigen}}$ remaining interactions are cancelled in the new method. Such is indeed the case for the comparisons made below.

Given the renormalized couplings and derivatives at some point it is a simple matter to locate the fixed point $\{K^*\}$ in a recursive fashion by use of the first order Taylor series expansion,

$$(K'_\alpha - K^*_\alpha) \simeq (\partial K'_\alpha/\partial K_\beta)(K_\beta - K^*_\beta), \tag{13}$$

which is valid near the fixed point. The known values of $\{K\}$ and $\{K'\}$ and their derivatives are inserted, and eq. (13) is solved for $\{K^*\}$. At this approximate value for K^* the process is repeated. Typically the fixed point is reached within one or two iterations from a reasonable starting point.

At the fixed point the critical exponents are cal-

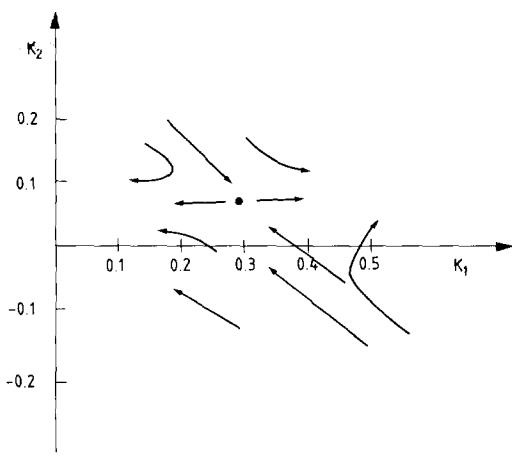

Fig. 2. Qualitative plot of flow diagram for the two-dimensional Ising model in the space at nearest neighbour (K_1) and second neighbour (K_2) couplings.

Table 1
Thermal exponent y_T of the two-dimensional Ising model, as calculated by the two methods described in the text (exact value $y_T = 1$).

	$K = (0.44068, 0.)$	$K^* = (0.32, 0.07)$
new method (2 × 2)	0.94	0.99
standard method (7 × 7 → 2 × 2)	0.95	0.96

culated by diagonalizing the appropriate derivative matrix. For example, if λ_e is the largest eigenvalue of the derivative matrix D of even-spin interactions, the thermal exponent y_T is given by

$$y_T = \ln(\lambda_e)/\ln 3. \quad (14)$$

The factor 3 arises because it is the scale factor for the block transformation. For the two-dimensional Ising model, y_T is exactly one.

3.2. Results. In the exercise we have chosen, the two-dimensional Ising model with majority rule blocking, a reasonable thermal exponent can be obtained by considering only the couplings K_1 and K_2. The resulting flow diagram is plotted in fig. 2. Note that there is a fixed point at $K^* = (0.32 \pm 0.01, 0.07 \pm 0.01)$. Here the errors are assessed by comparing the results of a block configuration with those of its negative. These values are consistent with those given in ref. [10].

The calculations were performed using a square lattice with 45 sites on a side. Correlations were measured over 90000 updates of the entire lattice after equilibration for 10000 updates. At the Ising model fixed point, $K \approx (0.44068, 0.)$, the value of the thermal exponent was found to be $y_T \approx 0.94$.

At the improved fixed point, $K^* \approx (0.32, 0.07)$, the thermal exponent was found to be $y_T \approx 0.99$. Note that knowledge of the truee fixed point can result in an improved value of the critical exponent (recall that the exact value is $y_T = 1$). For this calculation, the 2 × 2 matrix D involving derivatives of K_1' and K_2' was determined by our new method. As can be seen in table 1, these results are equivalent to those obtained by the standard method [2] using $N_{corr} = 7$ and $N_{eigen} = 2$. In the latter case the additional couplings involved included the third neighbor two-spin coupling and several four-spin couplings with two first neighbors and a second neighbor. All of these extra five couplings are cancelled in our new procedure; thus (as discussed above) the comparison is fair.

4. Conclusions

We have presented a method which can be used to find fixed points and coupling constant trajectories within the framework of the Monte Carlo renormalization group. The method is applicable to a wide variety of models, and can be used to determine trajectories even far from the critical point. Previous methods (see, e.g., ref. [5]) only determined trajectories in the neighborhood of a fixed point.

A new method for extracting directly the derivatives of the block renormalized couplings with respect to the original (site) couplings was also discussed. It was shown that knowledge of the critical point in the multiparameter space leads to an improved value of the thermal exponent, at least in the case considerd. We are presently applying the method to a Monte Carlo renormalization group study of ϕ^4 field theory.

Note added. At the conclusion of this research we learned of recent work [11] on a different method to extract block renormalized couplings.

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