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TITLE: IMPROVED MONTE CARLO RENORMALIZATION GROUP METHOD

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IMPROVED MONTE CARLO RENORMALIZATION GROUP METHOD

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An extensive program to analyse critical systems using an Improved Monte Carlo Renormalization Group Method (IMCRG)[1] being undertaken at LANL and Cornell is described. Here we first breifly review the method and then list some of the topics being investigated.

1) INTRODUCTION TO *MCRG*

Renormalization Group (RG) [2] is a general framework for studying systems near their critical point where all length scales are important. The scaling properties associated with second order phase transitions and the universal critical exponents have been calculated for many systems either analytically or by the Monte Carlo RG (*MCRG*) [2,3,4,5] method. The idea is as follows: Consider a magnetic system consisting of spins $\{s\}$ on the sites of a $d-dimensional$ lattice L described by a Hamiltonian H with all possible couplings $\{K_\alpha\}$. All thermodynamic quantities can be found from a detailed knowledge of the partition function

$$Z = Tr\, e^{-H} = Tr\, e^{K_\alpha S_\alpha} \tag{1}$$

where S_α are the interactions.

In the standard *MCRG* method [3,4,5,6], the spin configurations are generated with the Boltzmann factor e^{-H}. The renormalized theory -- interaction of block spins $\{s^1\}$ defined on the sites of a sublattice L^1 with lattice spacing b times that of L -- is defined by

$$e^{-H^1(s^1)} = Tr\, P(s^1, s)\, e^{-H(s)} \tag{2}$$

where the projection operator $P(s^1, s)$ (also called the renormalisation group transformation (*RGT*)) should integrate out the short distance fluctuations but leave the long distance physics unchanged. It satisfies the constraint

$$Tr^1\, P(s^1, s) = 1 \tag{3}$$

independent of the state $\{s\}$. This guarantees that the two theories have the same partition function.

Renormalisation group is the study of the transformation $H^1 = R(H)$ defined on the space of coupling constants, $\{K_\alpha\}$, of the model. At all fixed points H^* which have a divergent correlation length, the theory is scale invariant. This is the source of the scaling functions observed in thermodynamic systems. A certain

neighborhood, the set of critical points in the coupling space, forms the domain of attraction of the fixed point. The long distance physics of all theories attracted by a given fixed point is the same and under a *RGT* a critical Hamiltonian flows to the fixed point with the rate of flow given by the irrelevant eigenvalues. The relevant eigenvalue(s) give the rate of flow away from the fixed point (along the unstable direction) and are related to the critical exponent(s) ν. In the standard *MCRG* method [6] these are calculated from the eigenvalues of the linearized transformation matrix $T^n_{\alpha\beta}$ which is defined to be

$$T^n_{\alpha\beta} = \frac{\partial K^n_\alpha}{\partial K^{n-1}_\beta} = \frac{\partial K^n_\alpha}{\partial \langle S^n_\sigma \rangle} \frac{\partial \langle S^n_\sigma \rangle}{\partial K^{n-1}_\beta} \quad . \tag{4}$$

Each of the two terms on the right is a connected 2-point correlation function

$$\frac{\partial \langle S^n_\sigma \rangle}{\partial K^{n-1}_\beta} = \langle S^n_\sigma S^{n-1}_\beta \rangle - \langle S^n_\sigma \rangle \langle S^{n-1}_\beta \rangle . \tag{5}$$

and

$$\frac{\partial \langle S^n_\sigma \rangle}{\partial K^n_\beta} = \langle S^n_\sigma S^n_\beta \rangle - \langle S^n_\sigma \rangle \langle S^n_\beta \rangle . \tag{6}$$

Here $\langle S^n_\sigma \rangle$ are the expectation values on the n^{th} renormalized lattice and K^n_σ are the corresponding couplings. The exponent ν is found from the leading eigenvalue λ of $T^n_{\alpha\beta}$ as

$$\nu = \frac{\ln b}{\ln \lambda} \tag{6}$$

where b is the scale factor of the *RGT*. The accuracy of the calculated exponents improves if they are evaluated close to the fixed point. This can be achieved by starting from a critical point and blocking the lattice a sufficient number of times. The convergence is therefore limited by the starting lattice size and can be improved if H^n is used in the update. Thus it is important to determine the renormalized couplings $\{K^n\}$. The Achilles heel of this method is that as yet no way is known to determine the errors in the exponents obtained from a truncated set of matrices.

2) IMPROVED *MCRG*

In the Improved *MCRG* method the configurations $\{s\}$ are generated with the weight

$$P(s^1, s) e^{-H(s) + H^0(s^1)} \tag{7}$$

where H^0 is a guess for the H^1. Using both site and block couplings eliminates the long time correlations due to a divergent correlation length. If $H^0 = H^1$, then the block spins are completely uncorrelated and

$$\langle S^1_\alpha \rangle = 0 \qquad \langle S^1_\alpha S^1_\beta \rangle = n_\alpha \delta_{\alpha\beta} \tag{8}$$

where for the Ising model (and most other models) the integer n_α is simply a count of the number of terms (multiplicity) of interaction type S_α. When $H^0 \neq H^1$, then to first order

$$\langle S^1_\alpha \rangle = \langle S^1_\alpha S^1_\beta \rangle_{H^0 = H^1} (K^1 - K^0)_\beta \tag{9}$$

and using Eq. (8), the renormalized couplings $\{K^1_\alpha\}$ are determined with no truncation errors as

$$K^1_\alpha = K^0_\alpha + \frac{\langle S^1_\alpha \rangle}{n_\alpha} \quad . \tag{10}$$

This procedure can be iterated using H^{n-1} as the spin H in Eq. (7) to find H^n. If the irrelevant eigenvalues are small, then after two or three repetitions of the *RGT*, the sequence H^n converges to the fixed point

the update. This second limitation can be avoided by the following modification that allows a direct calculation of the n^{th} renormalized Hamiltonian H^n. In Eq. (7) use H^0 as the guess for H^n. The update now involves the original spins and the n^{th} *level* block spins in the Boltzmann weight

$$P(s^n, s^{n-1}) \ldots\ldots P(s^1, s) e^{-H(s)+H^0(s^n)} \quad . \tag{11}$$

The three Eqs. (8-10) are unchanged except that the *level* superscipt is replaced by n, i.e. the n^{th} *level* block-block correlation matrix is diagonal and given by Eq. (8). With this modification, the only limitation left is the size of the starting lattice.

The calculation of the *LTM* proceeds exactly as in the standard *MCRG* i.e. Eqs. (4) to (6). However, in the limit $H^0 = H^1$, the block-block correlation matrix is diagonal and given by Eq. (8). Thus it has no truncation errors, can be inverted with impunity and the final *LTM* elements are also free of all truncation errors. The only error is in finding the eigenvalues of a truncated matrix. A perturbation theory method to correct this error is described in [8].

To summarize, we find that simulating the system with several couplings and with both the block and site spins does complicate the program but there are three very important advantages of this method:

(1) Generating configurations according to Eq. (7) removes the long time correlations, so there is a very large gain in statistics, i.e. thermal equilibrium is reached quickly and the correlation between successive sweeps is limited to a few ($O(1)$) passes .

(2) The hardest part of such methods, an accurate calculation of $\langle S^1_\alpha S^1_\beta \rangle$ for many long range interactions, is known exactly. Also in the evaluation of the H^1 and *LTM*, a truncation in the coupling constant space does not affect the results because this matrix is diagonal.

(3) This method extends easily to Lattice Gauge Theories and other spin models [9].

3) CURRENT PROJECTS

1) To find the fixed points for the d=2 and d=3 Ising models.

2) To investigate the effect of tuning the RGT. The important question here is : Is the fixed point moved along the redundant directions only when the RGT is changed? If so, can the calculation of the critical exponents be improved by tuning the RGT.

3) To obtain the parameters of the effective field theories obtained by applying IMCRG to non-abelian gauge theories.

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