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Canonical Demon Monte Carlo Renormalization Group

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Abstract

We describe a new method to compute renormalized coupling constants in a Monte Carlo renormalization group calculation. The method can be used for a general class of models, e.g., lattice spin or gauge models. The basic idea is to simulate a joint system of block spins and canonical demons. In contrast to the Microcanonical Renormalization Group invented by Creutz et al. our method does not suffer from systematical errors stemming from a simultaneous use of two different ensembles. We present numerical results for the $O(3)$ nonlinear σ-model.

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1 Introduction

The Monte Carlo Renormalization Group (MCRG) [1] combines ideas of the block spin renormalization group (RG) and Monte Carlo (MC) simulations. In the classical MCRG one does not actually compute the flow of effective actions (Hamiltonians) or coupling constants, but instead uses the RG as a tool to define blocked observables that are suitable for the computation of critical properties. Examples for these techniques are the methods for the determination of critical exponents from the linearized RG transformation [2] and the matching method for the calculation of the $\Delta\beta$ function [3].

However, it would be more in the original spirit of the RG to really perform the integrations over the short wavelength degrees of freedom step by step in order to eventually come close to a fixed point or to arrive at a correlation length of order one. The price to pay for this is that one has to deal with a possibly complicated action with many coupling constants which in addition is not easy to compute. Furthermore, little is known on the effect of the truncations that one has to perform in the number couplings.

In the history of MCRG, some methods have been invented that allow to compute renormalized couplings with the MC method, some restricted to specific models, some more generally applicable. For a review on these methods see [4].

Creutz et al. have invented a method for the calculation of renormalized couplings that uses a microcanonical demon simulation [5]. However, the method suffers from systematic errors due to the fact that the canonical and microcanonical ensemble are equivalent only on large lattices.

We here present a modification of the demon method that overcomes this disadvantage. Our method does not introduce systematic errors. It shares with the Creutz et al. method the nice feature that one needs just a standard update program for its implementation.

2 Description of the Method

We consider a lattice spin system with spins ϕ_x. Denote the action of the spin system by S. The Boltzmann factor is $\exp(-S)$. Assume that the action can be parameterized by

$$S = -\sum_\alpha \beta_\alpha S_\alpha \,, \tag{1}$$

where S_α are interaction terms, and the β_α are real numbers. In addition we introduce an auxiliary system, called demon system, that is given by the action

$$S_D = \sum_\alpha \beta_\alpha d_\alpha \,, \tag{2}$$

where the β_α are the same as in eq. (1), and the d_α are real numbers in the interval $[0, d_{max}]$. In the following we shall consider the joint partition function

$$Z = \left(\prod_\alpha \int_0^{d_{max}} \mathrm{d}\, d_\alpha \right) \int D\phi \, \exp(-S - S_D) \,. \tag{3}$$

The partition function factorizes in the partition function of the spin system and the partition functions of the single demons. Hence we can compute the distribution of the demon variables d_α. One gets

$$< d_\alpha >= \frac{1}{\beta_\alpha}\left(1 - \frac{\beta_\alpha d_{max}}{\exp(\beta_\alpha d_{max}) - 1}\right) \tag{4}$$

This relation can be numerically solved with respect to β_α.

Now let us consider the situation of a numerical RG transformation. We simulate the spin model with a known action, and apply a certain blocking rule to the configurations on the fine grid to produce block spin configurations on a coarser grid. By this procedure we get the blocked configurations with a probability distribution according to their Boltzmann weight, but without knowing the block effective action explicitly.

Our proposal how to find the effective action is to perform a simulation of the joint partition function given in eq. (3).

We assume that the action of the blocked spin system is well described by the ansatz given by eq. (1). The simulation consists of two steps (see figure).

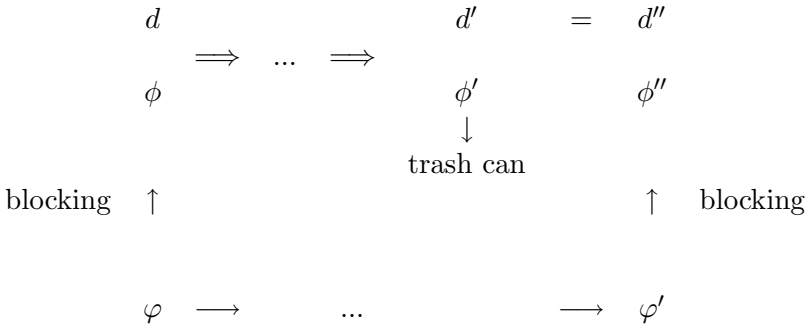

Figure: Scheme of our procedure to simulate the joint system of block spins and demons. The symbol $\Longrightarrow$ denotes the microcanonical updating of block spins ϕ and demons d, the symbol $\longrightarrow$ represents the standard updating of the fine grid spins φ.

1. Perform microcanonical updates of the joint system. These updates do not change the differences $S_\alpha - d_\alpha$. Since also the Boltzmann weight is unchanged, knowledge of the β_α is not required for the update.

2. Replace the block spin configuration by a new, statistically independent one.

The second step is ergodic and fullfils detailed balance if the simulation of the system on the fine grid satisfies these conditions. Statistical independence of the block configurations can be assumed if the configurations are sufficiently well separated in computer time, i.e., if the number of sweeps between two subsequent configurations is much larger than the autocorrelation time of the update algorithm for the fine grid spins.

One may ask whether the statistical independence of the block spin configurations is really necessary. We studied an exactly solvable toy model and found that correlated block spin configurations deteriorated the results.

It remains to show that spin-demon update step is ergodic for the demons. For the concrete update procedure to be described below, this property is not too difficult to show.

3 Numerical Results

We implemented the new method for the $O(3)$ invariant vector model in two dimensions. In particular we considered an action with 12 interaction terms,

$$S = -\sum_{\alpha=1}^{12} \beta_\alpha \sum_x S_{x,\alpha}\,, \tag{5}$$

where

$$S_{x,\alpha} = \tfrac{1}{2} \sum_{y \in Y_{x,\alpha}} (s_x \cdot s_y)^n\,. \tag{6}$$

The s_x are 3-vectors of unit length, and the $\cdot$ denotes the usual scalar product. The sets $Y_{x,\alpha}$ consist of all lattice points that can be obtained by the obvious symmetry operations from a representative lattice vector v, and n takes values in $\{1, 2, 3\}$. Table 1 gives n and v for $\alpha = 1...12$.

α	1	2	3	4	5	6	7	8	9	10	11	12
v	1,0	1,1	2,0	2,1	3,0	1,0	1,1	2,0	2,1	3,0	1,0	1,1
n	1	1	1	1	1	2	2	2	2	2	3	3

Table 1: Labelling of the 12 interaction terms $S_{x,\alpha}$

As a first test of the method and the program we tried to reproduce the couplings on a given lattice. We simulated the model with some ad hoc chosen set of couplings on an 8^2 and a 16^2 lattice. The updates were performed using a tunable version of the overrelaxation algorithm. The demon-spin update can be described as follows. First, a new value for a single spin is proposed. The probability for the change is symmetric in the start value and the proposed value. Then one checks whether the demons d_α can put the changes of the S_α in their backpacks, i.e., whether the sums $d_\alpha + \Delta S_\alpha$ remain inside the allowed interval $[0, d_{max}]$ for all α. If that is the case the proposal for the spin is accepted, and the demons are updated to the new value. Otherwise spin and demons keep their values.

The spin configurations used for the replacement in the spin-demon simulation have to be separated by a number of update steps that is large compared with the autocorrelation time. In oder to avoid wasting too many spin configurations we employed 100 independent demon systems. Then we generated a sequence of spin configurations, where two successive configurations were separated by a number of sweeps N_s large compared to the autocorrelation time divided by 100. The replacement configurations for the 100 demon systems were then successively taken from this sequence. After a replacement of the spin configuration, we always performed one lattice spin-demon updating sweep. After a full cycle through the demon systems the measured demon values were averaged over the 100 systems and written to disk.

	couplings	$L = 8$	$L = 8$, trunc	$L = 16$	$L = 16$, trunc
β_1	1.30	1.3010(23)	1.1399(10)	1.2999(12)	1.1408(7)
β_2	0.35	0.3481(12)	0.2993(6)	0.3485(8)	0.3014(4)
β_3	0.01	0.0105(9)	– 0.0020(6)	0.0098(6)	– 0.0017(4)
β_4	0.02	0.0190(7)	0.0138(3)	0.0192(4)	0.0149(2)
β_5	0.004	0.0045(6)	0.0019(4)	0.0039(5)	0.0022(2)
β_6	– 0.200	– 0.2045(30)		– 0.2002(18)	
β_7	– 0.080	– 0.0808(21)		– 0.0808(12)	
β_8	– 0.020	– 0.0201(11)		– 0.0188(6)	
β_9	– 0.01	– 0.0086(6)		– 0.0085(4)	
β_{10}	– 0.005	– 0.0045(8)		– 0.0038(6)	
β_{11}	0.02	0.0248(26)		0.0220(14)	
β_{12}	0.01	0.0131(19)		0.0114(12)	
ξ	57.8(4)				36.7(2)

Table 2: Reproduction of the original coupling constants. The columns labelled by "trunc" give the result from a truncation to an action with 5 couplings only.

Our results are presented in Table 2. In addition to the reproduction of the 12 original couplings we studied the truncation to a subset of 5 couplings. The truncation experiment served for us as preparation for the renormalization group study, where one is always faced with the necessity to truncate the ansatz for the effective action.

For the $L = 8$ lattice we performed 20000 updates of the 100 demon systems, with $N_s = 1$. In the $L = 16$ case we made 10000 updates, also with $N_s = 1$. The results show that the method works nicely. Most of the couplings are reproduced within 1 sigma error bars.

The last line gives correlation length estimates for the original set of 12 couplings and also for the couplings obtained from the truncated ansatz. The correlation length estimates were computed using a single cluster algorithm on a lattice very large compared to the correlation length. The correlation length of the truncated coupling set is significantly smaller than the original one. A naive truncation of the original set of couplings (just

throwing away the couplings β_6 to β_{12}) gives a correlation length larger than 200. On an $L = 400$ squared lattice we measured $\xi = 195.5 \pm 2.3$.

Next we studied renormalization group transformations, starting from the standard action with nearest neighbour coupling only. We used a blocking rule that we call "dressed decimation". All lattice points that have coordinates $x = (i, j)$ with i *and* j even are identified with block sites. The block spin s' at site x is then defined as

$$s'_x = \frac{w s_x + \frac{1}{4}(1-w)\sum_{y.nn.x} s_y}{|w s_x + \frac{1}{4}(1-w)\sum_{y.nn.x} s_y|}\,, \tag{7}$$

where the sum is over the nearest neighbours of x. Tests with the massless free field theory revealed that the choice $w = 0.8$ is a good one in the sense that the effective actions and especially the fixed point action had good locality properties.

As a first test we started with $\beta_1 = 1.9$, and all the other couplings put to zero. The correlation length for this coupling is 121.2(6) [6]. We applied the blocking rule described above to generate the block configuration used in the replacement step for the demons. We always blocked a 32^2 lattice down to 16^2 lattice. The effective couplings within the truncation scheme of the 12 couplings given above were then determined from the demon expectation values. The effective couplings were then used as input for the next iteration step. Our results for the first 4 steps are presented in Table 3. In the last line we give again correlation length estimates for the effective theories, again obtained with a single cluster algorithm on huge lattices.

Note that in case of an exact renormalization transformation the correlation length should change exactly by the scale factor of the blocking rule, that in our case is two. The strong deviations that we observe clearly indicate that one should include more couplings in the ansatz for the effective action.

Note also that there is a very good decay of the couplings with given n with increasing distance of the spins. We conclude from this and the systematic errors in the correlation lengths that probably local interactions with higher n and also interactions with more than two spins cannot be left out. (E.g., 4-point operators proved to be important in the study of Hasenfratz et al. [7] using the classical approximation.) Careful studies of these issues, also using alternative methods for the determination of the effective couplings and other blocking rules are underway [8].

RG step	0	1	2	3	4
β_1	1.9	1.4619(15)	1.1764(11)	0.9785(16)	0.8201(14)
β_2	0.0	0.2691(9)	0.3117(8)	0.2892(8)	0.2528(8)
β_3	0.0	– 0.0123(6)	0.0107(5)	0.0226(6)	0.0272(4)
β_4	0.0	0.0074(4)	0.0132(3)	0.0182(3)	0.0195(4)
β_5	0.0	0.0043(5)	0.0031(4)	0.0032(5)	0.0034(4)
β_6	0.0	– 0.2213(19)	– 0.2611(13)	– 0.2257(14)	– 0.1689(12)
β_7	0.0	– 0.0800(12)	– 0.1027(10)	– 0.0985(13)	– 0.0766(9)
β_8	0.0	0.0003(9)	– 0.0057(6)	– 0.0104(7)	– 0.0107(8)
β_9	0.0	– 0.0022(5)	– 0.0011(5)	– 0.0077(5)	– 0.0081(5)
β_{10}	0.0	– 0.0005(6)	– 0.0011(5)	– 0.0014(7)	– 0.0015(7)
β_{11}	0.0	0.0659(17)	0.0898(13)	0.0748(18)	0.0470(15)
β_{12}	0.0	0.0327(13)	0.0440(11)	0.0425(15)	0.0301(12)
ξ	121.2(6)	57.0(4)	24.5(2)	10.47(5)	4.78(2)

Table 3: Results for the first four RG steps, starting from the standard action with $\beta_1 = 1.9$. The last line gives the correlation lengths for the effective theories. The successive columns give the results of the subsequent RG steps.

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