Microcanonical Renormalization Group

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We argue that microcanonical Monte Carlo techniques can provide direct information on the values of renormalized coupling constants in numerical renormalization-group studies. The method is tested on SU(2) lattice gauge theory with fundamental and adjoint couplings and on the two-dimensional O(3) Heisenberg model.

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In this Letter we present some results obtained on a new method of determining renormalized coupling constants in a Monte Carlo renormalization-group (RG) calculation. The method is quite general in that it can be applied to any model with (at least in principle) any number of coupling constants. The Monte Carlo RG combines the ideas of the block-spin RG and Monte Carlo simulations.[1] Typically, one creates an ensemble of configurations with a weight proportional to some initial Hamiltonian, then blocks the spins according to some RG rule. The new ensemble of block-spin configurations thus obtained would be distributed according to the new renormalized Hamiltonian. Then, once the renormalized Hamiltonian is explicitly determined, one can study the coupling-constant flow under rescaling, find critical exponents near a RG fixed point, and determine the β function of the theory in a regime of coupling-constant space that is not accessible to any kind of perturbative treatment. The last step above (finding the renormalized Hamiltonian) has traditionally been the most problematic one, involving complicated matching procedures. Recently new methods to find renormalized couplings have been developed.[2] However, they are very different from what is proposed here.

Our method of finding renormalized couplings is simple: It is a basic feature of a simulation of the microcanonical ensemble[3-4] that the coupling constants of a given Hamiltonian do not serve as input but are rather a result of the computation. The strategy then is to simulate some Hamiltonian, perform the blocking, and use the block-spin configuration thus obtained as an input for a microcanonical simulation. The result of the latter simulation will be the values of the renormalized coupling constants. In the implementation of the microcanonical ensemble in Ref. 4, one simulates the "partition function"

$$Z_{\mathrm{MC}}=\sum'_{E_D}\sum_C\delta[H(C)-E_D-E_0]. \tag{1}$$

Here E_0 is the total energy which is held constant during the simulation; E_D refers to the energy of an extra degree of freedom (the "demon") which hops through the lattice and attempts to update the variables of the problem. The sum in (1) is over configurations and properly constrained demon energies. Standard statistical mechanical arguments suggest that for a large system the demon's energy will be distributed according to Boltzmann's law:

$$P(E_D)\propto e^{-\beta E_D}. \tag{2}$$

Hence if, for example, E_D is restricted to $E_D>0$, the inverse temperature β ("coupling constant") is given by

$$\beta=1/\langle E_D\rangle. \tag{3}$$

In a RG calculation several couplings must be determined simultaneously. This can be done in the following way: Suppose our system of interest is governed by the canonical partition function

$$Z=\sum_C\exp[-\sum_i\beta_i H_i(C)]. \tag{4}$$

Then the appropriate microcanonical partition function is

$$Z_{\mathrm{MC}}=\sum_{\{E_{D_i}>0\}}\sum_C\prod_i\delta[H_i(C)+E_D^i-E_0^i], \tag{5}$$

$$\beta_i=1/\langle E_D^i\rangle. \tag{6}$$

This corresponds to having one demon carry as many sacks as there are coupling constants—each one labeled by the index i in (5). (E_D^i therefore is the energy in the ith sack; E_0^i is the total energy

corresponding to H_i.) If some of the coupling constants can be negative, one must constrain the demon energy to lie in some finite interval $[-E_M, E_M]$. In this case one obtains instead of (6) the invertible relation

$$\langle E_D^i \rangle = 1/\beta_i - E_M/\tanh\beta_i E_M. \quad (7)$$

As a single demon carries only a small fraction of the system energy, its initial value is unimportant. This is in contrast to a conventional molecular-dynamics version of microcanonical simulation, wherein each degree of freedom has an independent conjugate momentum.[3] Furthermore, a molecular-dynamics approach would not allow simultaneous determination of several couplings.

TABLE I. Determination of fundamental and adjoint couplings in SU(2) lattice gauge theory.

Monte Carlo	β_F	β_A
$(2,-0.5)$	1.999 ± 0.003	-0.486 ± 0.004
$(3,1)$	3.08 ± 0.03	0.99 ± 0.02
$(0.5,0.5)$	0.495 ± 0.002	0.501 ± 0.002

Relations (6) and (7) have finite-volume corrections of the form[5]

$$\langle E \rangle_v = \langle E \rangle_\infty + (2CV)^{-1}(\langle E \rangle_\infty \langle E^2 \rangle_\infty - \langle E^3 \rangle_\infty) + O((2CV)^{-2}). \quad (8)$$

They are especially small near a critical point where the specific heat C of the system becomes large. Furthermore, they are also small at weak coupling or large β [$O(1/\beta^3)$]. The inherent statistical error in a determination of β_i via (3) and (6) is of order $O(\beta_i)$ per measurement of E_D. This statistical error can be made arbitrarily small by performing sufficiently long runs.

We have studied the method on different models: SU(2) gauge theory with a mixed fundamental-adjoint action[6] and the O(3) Heisenberg model in two dimensions. For the gauge case we merely present the determination of (β_F, β_A) on an 8^4 lattice at three different values of the couplings. We first prepare a thermalized configuration via conventional Monte Carlo methods. Then starting from this configuration we performed 300 microcanonical iterations with the initial demon energies set to $E_D^i = 0$. The central values and errors shown in Table I refer to this one particular configuration. A better procedure is to prepare a configuration with an energy equal to the *average* energy of a number of initial Monte Carlo configurations. This procedure was followed in the O(3) case. We studied the following O(3)-symmetric three-coupling Hamiltonian

$$\sum \beta_i H_i = \beta_1 \sum_{n,\mu}(1 - \vec{S}_n \cdot \vec{S}_{n+\mu}) + \beta_2 \sum_n (2 - \vec{S}_n \cdot \vec{S}_{n+x+y} - \vec{S}_n \cdot \vec{S}_{n+x-y}) + \beta_3 \sum_{n,\mu}(1 - \vec{S}_n \cdot \vec{S}_{n+2\mu}). \quad (9)$$

TABLE II. Expectation values of internal energies of block spins and renormalized coupling constants. The errors are the statistical errors obtained from individual Monte Carlo runs.

Size, β	Block size	F_1	E_2	E_3
128×128,	1	0.4907 ± 0.0001	0.6159 ± 0.0001	0.6913 ± 0.0001
$\beta_1 = 1.28$	2	0.5046 ± 0.0001	0.6490 ± 0.0002	0.7668 ± 0.0005
	4	0.6095 ± 0.0008	0.7712 ± 0.0006	0.8832 ± 0.0009
	8	0.7557 ± 0.0017	0.9036 ± 0.0036	0.9748 ± 0.0041
64×64,	1	0.5906 ± 0.0001	0.7318 ± 0.0001	0.8049 ± 0.0001
$\beta_1 = 1.064$	2	0.6435 ± 0.0002	0.7950 ± 0.0002	0.8946 ± 0.0004
	4	0.7622 ± 0.0005	0.9031 ± 0.0005	0.9741 ± 0.0013
		β_1	β_2	β_3
128×8,	1	1.285 ± 0.008	0.006 ± 0.005	0.008 ± 0.004
$\beta_1 = 1.28$	2	1.486 ± 0.017	0.002 ± 0.004	-0.200 ± 0.012
	4	1.232 ± 0.010	-0.019 ± 0.005	-0.196 ± 0.012
	8	0.758 ± 0.007	-0.020 ± 0.006	-0.111 ± 0.004
64×64,	1	1.060 ± 0.007	-0.001 ± 0.007	0.002 ± 0.009
$\beta_1 = 1.064$	2	1.041 ± 0.009	0.019 ± 0.010	-0.123 ± 0.008
	4	0.727 ± 0.005	-0.002 ± 0.003	-0.099 ± 0.009

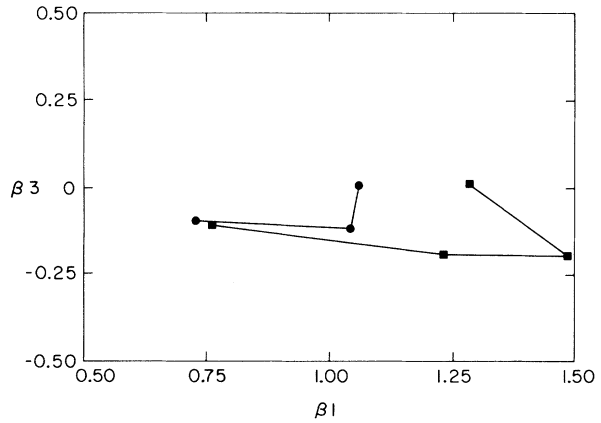

FIG. 1. After three blockings, the trajectory starting from a 128×128 lattice (squares) reaches the twice-blocked trajectory starting from a 64×64 lattice (circles).

Here n is a lattice site and μ a unit vector in the lattice. We determined the RG flows of coupling constants starting from the two points (1.28,0,0) and (1.064,0,0). In the work of Shenker and Tobochnik[7] these two points were determined to have correlation lengths differing by a factor of 2. Our results are summarized in Table II. We first evaluated the three internal energies of the block spins $E_i \equiv \langle H_i \rangle$ using ordinary Monte Carlo methods. At $\beta_1 = 1.28$ we used a 128×128 lattice and averaged over 2400 iterations. At $\beta_1 = 1.064$ a 64×64 lattice was used and 12 000 iterations performed. Then a new configuration having the averaged blocked internal energies E_i was prepared. This configuration was used as a start for a microcanonical simulation with all the demon energies restricted to lie in the interval $[-1, 1]$. To minimize finite-size effects the lattice size of the microcanonical runs was always that of the blocked lattice. The number of microcanonical iterations we performed was $8000\times(16/L)^2$, where L is the linear size of the blocked lattice. From our data it is clear that the coupling constants of the two initial lattices approach each other after, respectively, three and two blockings (Fig. 1). This indicates that the initial couplings do indeed correspond to Hamiltonians with correlation length ξ and $\xi/2$, thus confirming the results of Ref. 7.

To summarize, we have proposed a new numerical method to evaluate renormalized coupling constants. Its main advantage is that it is fast and extremely easy to implement.

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