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THE EFFECTIVE ACTION FROM MULTIGRID MONTE CARLO*

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We describe a new method to calculate the effective action in lattice field theories through the multigrid Monte Carlo technique. It permits stochastic computations for critical and nearly critical systems without critical slowing down. As a first application the ϕ^4-theory in 4 dimensions with spontaneous symmetry breaking is studied. We obtain an estimate of the dynamical critical exponent. The strong reduction of the relaxation time permits accurate determination of the effective action close to the critical surface.

1. INTRODUCTION

The basic idea of the multigrid approach is to map a nearly critical lattice field theory into a noncritical theory which lives on a multigrid. In effect one performs simultaneously a sequence of renormalization group transformations[1].A previous implementation[2] of this proposal did not minimize the coupling to high frequency fields, but renormalization theory shows that this is essential to get a noncritical system[3].

We present here a new Multigrid Monte Carlo algorithm which is motivated by analytical investigations and apply it to the ϕ^4 model with spontaneous symmetry breaking in 4 dimensions. Our scheme is designed for moderate couplings. We believe that moderately strongly coupled models are of prime interest because very strongly coupled models tend to become moderately coupled very quickly in initial renormalization group steps.

2. MULTIGRID DECOMPOSITION

To study a theory on the fundamental lattice Λ_N, called *base*, of lattice spacing $a = a_N$, we introduce a multigrid $\Lambda = \Lambda_0 + \Lambda_1 + ... + \Lambda_N$. It is composed of a sequence of lattices Λ_j, called horizontal layers, of decreasing lattice spacings $a_j = L^{N-j}a_N$, $L = 2$ or 3. We set $a_N = 1$. The multigrid may be regarded as a kind of lattice in one more dimension. The idea is to transform a nearly critical system in a box on *base* into a noncritical system on Λ. A linear multigrid transformation is similar to a Fourier transformation. It maps a field ϕ on the fundamental lattice *base* into a field φ on the multigrid Λ. For instance

$$\phi(z) = \sum_{j=0}^{N} a_j^{-d} \sum_{x \in \Lambda_j} A^j(z,x)\varphi^j(x) \quad (2.1)$$

in d dimensions. Sites $x \in \Lambda_j$ may be identified with cubes of sidelength L lattice spacings in Λ_{j+1}, and with cubes called *blocks* of sidelength L^{N-j} lattice spacings in *base*. Given the real kernels $A^j(z,x)$ - they are analogous to $\exp(ikx)$ in a Fourier transformation - the decomposition (2.1) is unique if one requires that the average of $\varphi^j(x)$ over cubes $y \in \Lambda_{j-1}$ of side La_j vanishes. There are then equally many independent variables $\phi(z)$ and $\varphi^j(x)$.

The essential steps in a renormalization group approach are
i) definition of a sequence of block spins $\Phi^j(x)$ on the lattices Λ_j, e.g. as block averages

$$\Phi^j(x) = av_{z \in x}\phi(z) \quad for \quad x \in \Lambda_j (z \in base) \quad (2.2)$$

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ii) a split of the fundamental field ϕ into a term called background field which is determined by the block spin Φ^j, and a fluctuation field ζ^j. Both fields live on *base*, and the fluctuation field contributes nothing to the block spin i.e. has zero block averages

$$\phi(z) = a_j^d \sum_{x \in \Lambda_j} A(z,x)\Phi^j(x) + \zeta^j(z) \,. \qquad (2.3)$$

Given the block spin definition (2.2) and the kernels A^j, eq.(2.3) defines the fluctuation field ζ^j as a function of ϕ.

The multigrid transformation (2.1) yields such a decomposition (2.3) for each j if we require that

$$av_{z \in y} A(z,x) = a_j^{-d}\delta_{xy} \qquad \text{for} \qquad x,y \in \Lambda_j \, (2.4)$$

and if A^j is constructed as convolution of kernels $A^{k,k-1}(x,y)$ which link neighbouring layers $\Lambda_k \ni x$ and $\Lambda_{k-1} \ni y$, and which share a property like (2.4). The fluctuation field $\zeta^k(z)$ equals the sum of terms in eq.(2.1) with $k \geq j+1$, and the background field is the rest. Thus the block spin receives contributions from φ^j on layers $j \leq k$ with lattice spacings $a_j \geq a_k$.

In the updating procedure one uses block spins Φ^j and fluctuation fields ζ^j, but for the following discussion of the requirements for noncriticality the multigrid transform $\phi \mapsto \varphi$ is essential. It maps a lattice field theory on *base* with Hamiltonian $\tilde{H}$ into a theory on Λ with Hamiltonian H,

$$\tilde{H}(\phi) = H(\varphi) \qquad (2.5)$$

This system will be noncritical if a variable $\varphi^j(x)$ attached to one site $x \in \Lambda$ has sizable correlations with a reasonably small number of variables $\varphi^k(y)$ only.

Assuming the kernel $A^j(z,x)$ is smooth in z on length scale a_j, the contribution of the field φ^j to ϕ shall represent the contribution from a certain frequency range. Therefore the conditional probability distribution $\exp[-\ldots(\varphi)]d\varphi^j$ for φ^j, given the fields φ^k on other layers $k \neq j$, is given by an auxiliary theory on Λ_j, with both an UV-cutoff a_j^{-1}, and also an infrared cutoff a_{j-1}^{-1} for $j \neq 0$. One can therefore expect that this auxiliary theory will only have correlation length of order a_{j-1}, that is L lattice spacings on Λ_j. This is confirmed by the renormalization group interpretation of the multigrid transform. In principle, the correlation length on Λ_0 equals that of the full theory, but our Λ_0 will be a single point.

This is not the complete story yet. In the full theory there are correlations between layers. For instance, a $\phi^4(z)$ interaction couples fields $\varphi^{j_1} \ldots \varphi^{j_4}$ on possibly different layers, by eq.(2.1),(2.5).The kernels $A^j(z,x)$ are chosen to decay exponentially in the distance $|z-x|$ of z from cube x, with decay length a_j. Therefore they introduce nonlocality in horizontal direction over distances a_j only.But for $k > j$ the number of points y in Λ_k "underneath" $x \in \Lambda_j$ - that is within horizontal distance a_j - increases exponentially with $k-j$ like $L^{d(k-j)}$. Therefore the coupling between layers Λ_j and Λ_k with $k > j$ could induce correlations in Λ_k over distances of order L^{k-j} lattice spacings. This shows that noncriticality of the full theory can only be achieved if correlations between φ^j and fields φ^k which represent higher frequency ranges $k > j$, decay fast enough with $k-j$. Such decoupling between high frequency fields and low frequency fields is a subject of renormalization theory.

Rigorous analytical work [3] on renormalization group and phase cell cluster expansions showed for some weakly coupled models without spontaneous symmetry breaking that the theory on the multigrid admits convergent cluster expansions, and is therefore essentially noncritical, if one imposes the following requirements on the kernels $A^j(z,x)$:
i) relation (2.4) for block averages
ii) exponential decay in $|z-x|$ over distances a_j
iii) the kinetic term $(\phi, -\Delta\phi)$ does not couple different layers.

Because $\varphi^j(x)$ has vanishing averages over cubes $y \in \Lambda_{j-1}$, condition iii) is fulfilled if

$$-\Delta_z A^j(z,x) = const \qquad (2.6)$$

as a function of z on cubes $y \in \Lambda_j$. Step function kernels as employed by Goodman and Sokal [2] do not lead to a noncritical system.

3. MULTIGRID MONTE CARLO SIMULATION

We did numerical studies of the performance of such a scheme for moderate coupling, in the vicinity of a critical point (surface) and including points in the broken symmetry phase, for 1-component Φ^4 theory in 4 dimensions. The kernels A^j can be computed from eq.(2.6) by relaxation. One updates at pairs of points z_1, z_2 in the same cube to maintain eq.(2.4). The result showed that $A^j(z,x)$ is very small except if z is in cube x or in one of its nearest neighbours. Therefore we set it to zero elsewhere, for reasons of numerical simplicity. That is, we substituted a Laplacian with Dirichlet boundary conditions in eq.(2.6). The kernels A^j need to be computed only once.

The simulation was performed as follows. One visits the layers Λ_j in sequence; on $\Lambda_N = base$ one does standard Monte Carlo updates for ϕ. Before starting on Λ_j, $(j < N)$ one computes the fluctuation field ζ^j from the instantaneous field configuration ϕ by eq.(2.3). (ζ^j enters the kinetic term because of our truncation of A^j). One sweeps through sites $x \in \Lambda_j$, updating $\Phi^j(x)$, while ζ^j remains unchanged.

Updating Φ^j is essentially equivalent to update φ^j because the contributions of lower frequency fields φ^k $(k < j)$ will be changed by little,since only φ^j is not affected by critical slowing down. We make updating proposals for Φ^j based on the exact kinetic term which is bilinear in Φ^j and ζ^j, and filter with the exact interaction $\frac{1}{2}m_0^2\phi^2 + \lambda_0\phi^4$. This filtering is the costly step. It requires evaluation of the change of $\phi(z)$ for z in cube x and its nearest neighbours, and of the associated change in $\lambda_0 \sum \phi^4(z)$. As a result the amount of computational work on a block lattice Λ_j, $(j \neq 0)$ is comparable to that on the finest lattice Λ_N. Evaluation of the exact Hamiltonian cannot be avoided without introducing systematic errors in the probability distribution of ϕ.

Our last layer Λ_0 was chosen as a single point. As a result, the last block spin Φ^0 is a single real variable, and

$$\begin{aligned} \Phi^0 &= a_0^{-3} \cdot \text{magnetization} \\ \zeta^0(z) &= \phi(z) - \Phi^0 \,. \end{aligned} \tag{3.1}$$

The computations needed to update Φ^0 yield the effective action $\tilde{H_{eff}}(\Phi^0)$ for free. By definition

$$e^{-\tilde{H}_{eff}(\Phi^0)} = \int D\phi \, e^{\tilde{H}(\phi)} \, \delta\Big(\Phi^0 - a v_{z\in\Lambda_N} \phi(z)\Big) \tag{3.2}$$

The conditional probability distribution for Φ^0, given ζ^0, is $\propto \exp[-\tilde{H}(\Phi^0+\zeta^0]$,and for a ϕ^4 theory

$$\tilde{H}(\Phi^0 + \zeta^0) = \sum_{n=0}^{4} g_n(\zeta^0)\,(\Phi^0)^n \tag{3.3}$$

The updating procedure yields fluctuation field configurations ζ_a^0 with $a = 1...N_S$, N_S = number of visits. We compute and gather the corresponding fluctuating coupling constants $g_{n,a} = g_n(\zeta_a^0)$. They yield the effective action $\tilde{H_{eff}}(\hat{\Phi})$ and its derivatives with respect to $\hat{\Phi}$ as follows. Define Z_a as a 1-dimensional integral, and $g'_{n,a}(\hat{\Phi})$ by reexpanding,

$$\begin{aligned} Z_a &= \int d\Phi \exp\Big[-\sum_{n=0}^{4} g_{n,a}\Phi^n\Big] \\ \sum_{n=0}^{4} g_{n,a}\Phi^n &= \sum_{n=0}^{4} g'_{n,a}(\hat{\Phi})(\Phi - \hat{\Phi})^n \end{aligned}$$

Then we obtain

$$e^{-\tilde{H}_{eff}(\hat{\Phi}+\delta\Phi)} = N_S^{-1}\left[\sum_{a=1}^{N_S} Z_a^{-1} \exp\Big[-\sum_{n=0}^{4} g'_{n,a}(\hat{\Phi})(\delta\Phi)^n\Big]\right] \tag{3.4}$$

Expanding the logarithm on both sides in a power series in $\delta\Phi$ yields $\tilde{H_{eff}}(\hat{\Phi})$ and its derivatives. It costs little to do this for many $\hat{\Phi}$.

We used a multigrid $\Lambda_0 + \Lambda_1 + \Lambda_2$ to study single component ϕ^4 theory on a 12^4 lattice. Λ_1 had 4^4 sites, each representing a cube of 3^4 points, Λ^0 was a single point. We have also results on a 24^4 lattice.

We choose as bare input parameters for the coupling and mass the values $\lambda_0 = 16.376$ and $m_0^2 = -1.14, -1.15$ and -1.16 to study the expected crossover of the effective action from a single well shape to double well behaviour. Lüscher and Weisz[4] predicted that the critical point associated with second order phase transition for infinite volume is for this coupling at a bare mass $m_0^2 = -1.157 \pm 0.006$.

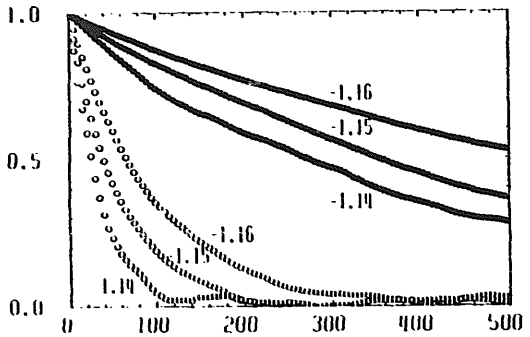

Figure 1: Autocorrelation function with Metropolis updating (filled circles) and the multigrid algorithm (open circles) on a 12^4 lattice.

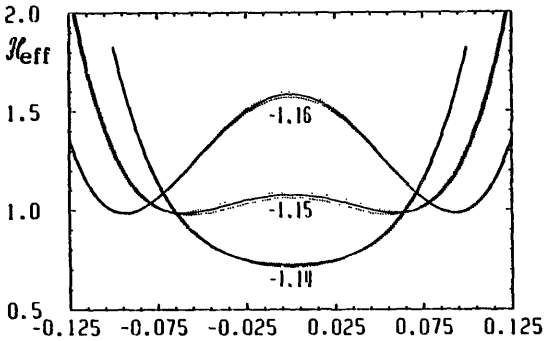

Figure 2: The effective action from the multigrid simulation on a 12^4 lattice as a function of the magnetization per site.

In our simulation we visited the multigrid layers in turn, performing 5 sweeps per visit with standard 50,20 and 10 hit Metropolis updates at each site for the three layers. Fluctuating coupling constants were determined once per visit. The effective action was computed from data samples of 200 000 sweeps, as described above, essentially without additional computational cost.

We made a comparison with the standard ("1-grid") Metropolis updating on the finest lattice. In figure 1 we compare the normalized time-autocorrelation function of the total magnetization for three values of the bare mass on a 12^4 lattice. Our data for $m_0^2 = -1.15$ on the 24^4 lattice are not plotted in fig.1 . The values for the autocorrelation time are $\tau = 400$, 550 and 800 for the three Metropolis runs and $\tau = 35$, 65 and 100 for the corresponding multigrid simulations. A change of the linear size L of the system from $L = 12$ to $L = 24$ increases the autocorrelation time τ from 65 to 100 at the bare mass $m_0^2 = -1.15$ which is very close to the infinite volume critical point. Therefore we can give an estimate $z_{MGMC} < 2$ for our multigrid Monte Carlo algorithm[5].

In figure 2 we show the total effective action $\tilde{H_{eff}}$ (*not* divided by the volume) in a narrow range of bare parameters with the crossover from a single well shape to double well behaviour. For $m_0^2 = -1.14$ the system is in the symmetric phase, at $m_0^2 = -1.15$ the symmetry is spontaneously broken (due to the finite size shift), and at $m_0^2 = -1.16$ we are clearly in the broken phase. The dotted lines are the errors of $\tilde{H_{eff}}$. Note the scale for $\tilde{H_{eff}}$.

One can determine renormalized coupling constants and masses m_r from the location of the minimum and derivatives of the effective action. Using the known value $Z \approx 1^4$ of the wave function renormalization constant we find $m_r = 0.10_5 \pm .01, 0.060 \pm .006, 0.16 \pm .01_5$ for $m_0^2 = -1.14, -1.15, -1.16$. This shows that we are very close to the critical point. We stayed so close in order to demonstrate the power of our method to fight critical slowing down.

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