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Overrelaxation Algorithm for coupled Gauge-Higgs Systems

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Abstract

In this letter we extent the overrelaxation algorithm, known to be very efficient in gauge theories, to coupled gauge-Higgs systems with a particular emphasis on the update of the radial mode of the Higgs field. Our numerical tests of the algorithm show that the autocorrelation times can be reduced substantially.

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1

The electroweak baryogenesis has attracted a lot of attention recently [1]. In order to understand this phenomenon a detailed description of the electroweak phase transition (PT) is needed. In its study it is sufficient to concentrate on the SU(2) group alone and to neglect all fermion fields and the U(1) subgroup. One therefore remains with a coupled system of gauge and Higgs fields which are elements of SU(2) and complex doublets, respectively. Although this so-called SU(2)-Higgs model has been investigated up to 2-loop order at finite temperature in perturbation theory by now [2], numerical simulations, which intrinsically contain also non-perturbative effects, are desirable. This is even more so as the 2-loop results showed large corrections to quantities like the surface tension as compared to 1-loop results. Therefore it seems necessary to confront the perturbative approach with numerical "experiments" to test the reliability of the perturbative results.

The Monte-Carlo simulations are necessarily done on a discretized (euclidean) space time lattice. To obtain results which are not distorted by the lattice one would like to go close to the continuum and work in the "scaling region". To approach this limit some of the correlation lengths ξ_i have to diverge. This causes the basic problem of all numerical simulations as with growing correlation lengths the problem of critical slowing down arises. In order to obtain independent configurations, suitable for measurements of physical quantities, one has to take into account the autocorrelation time which is the number of iterations with a given algorithm to reach a new independent configuration. The autocorrelation time grows with the correlation length as $\tau \propto \xi^z$ with z the so called dynamical critical exponent. For local algorithms like Metropolis or heatbath z is known to be 2. This implies that for ξ's of the order of 5-10, which are realistic values of todays simulations of the SU(2)-Higgs model, the autocorrelation time can be of the order of 25-100. Indeed, as will be shown below, in the SU(2)-Higgs model, for parameter values where one can compare results from perturbation theory and numerical simulations, the autocorrelation times are $O(100)$. This appears to be a major drawback for Monte-Carlo studies of the electroweak PT.

It is consequently not surprising that fighting critical slowing down is one of the major activities in the area of Lattice field theory. In fact, in the last few years several important steps have been done to solve this problem. Cluster [3] and multigrid [4] techniques are able to reduce critical slowing down almost completely, giving $z \approx 0$. However, these techniques are so far either only applicable for spin models (cluster) or did not lead to a big improvement in non-abelian gauge theories (multigrid).

For gauge theories another interesting approach, the overrelaxation method, as initiated by Adler [5] as a generalization of the heatbath algorithm seems to be most promising. In its popular limiting case the field evolution is deterministic and conserves energy (microcanonical).

In order to restore the necessary ergodicity one uses standard, ergodic updates (e.g. Metropolis or heatbath) and microcanonical updates alternately with a given mixing ratio. These so called hybrid algorithms turned out to be extremely efficient in pure gauge theories [6]. In this case the overrelaxation step is a kind of reflection of the local field with the following features:
a) the energy is unchanged
b) since the reflection is an element of the gauge group, the measure in the defining functional integral is invariant

2

We will extent this approach to coupled gauge-Higgs systems. Consider an SU(2) gauge-Higgs system with the following lattice action:

$$S = S_g + S_h, \tag{1}$$

where

$$S_g = -\frac{\beta}{2}\mathrm{Tr}(\sum_p U_p) \tag{2}$$

is the usual Wilson plaquette action and

$$S_h = -\kappa \mathrm{Tr}(\sum_{x,\mu} \Phi_x^\dagger U_{x,\mu} \Phi_{x+\mu}) + \sum_x \left[\Phi_x^\dagger \Phi_x + \lambda(\Phi_x^\dagger \Phi_x - 1)^2\right] \tag{3}$$

describes the self interaction of the four component Higgs field Φ_x and its coupling to the gauge field. Here one can introduce the standard 2×2 matrix notation, $\Phi_x = \rho_x \alpha_x$, where $\rho_x \in R$, $\rho_x \geq 0$, and $\alpha_x \in SU(2)$.

The reflection of the gauge field and the angular part of the Higgs field can be done analogously as for pure gauge fields and the above a) and b) conditions can be satisfied. However, for the radial part of the scalar field the reflection fulfills a) but not b), thus a careful treatment of the measure is needed in order to obtain a proper technique.

First we will study the microcanonical updating of the link variables. The action can be written as a sum of two terms: a term which contains the local link variable and a constant term.

$$S = \mathrm{Tr}(U_{x,\mu} V) + const, \tag{4}$$

where

$$V = -\frac{\beta}{2} \sum_{\nu \neq \mu, \nu \neq -\mu} U_{x+\mu,\nu} U^\dagger_{x+\nu,\mu} U^\dagger_{x,\nu} - \kappa \sum_\mu \rho_x \rho_{x+\mu} \alpha_{x+\mu} \alpha_x^\dagger. \tag{5}$$

Consider an update as a "reflection" of U

$$U'_{x,\mu} = V_0^\dagger U^\dagger_{x,\mu} V_0^\dagger, \tag{6}$$

where V_0 is the normalized V, thus $qV_0 = V$, where $q \in R$ and $V_0 \in SU(2)$. (Note the special feature of the $SU(2)$ group that the sum of several $SU(2)$ matrices with real coefficients is a product of a real number and an $SU(2)$ matrix.) As in the case of pure gauge theory it is easy to see that this updating satisfies the above mentioned a) and b) conditions.

The microcanonical updating of the angular part of the scalar field can be done completely analogously.

$$S = Tr(\alpha_x^\dagger V) + const, \tag{7}$$

where

$$V = -\kappa\rho_x \sum_\mu \rho_{x+\mu} U_{x,\mu} \alpha_{x+\mu}\,, \tag{8}$$

thus the updated angle

$$\alpha_x' = V_0 \alpha_x^\dagger V_0, \tag{9}$$

where V_0 is, as above, the normalized V. Again, one can show that the above a) and b) conditions are satisfied.

The most interesting case is the microcanonical updating of the radial mode of the scalar field. Separating the angular and the radial modes as $\Phi = \rho\alpha$, the $\mathcal{D}\Phi\mathcal{D}\Phi^\dagger$ measure will get a form of $d\alpha d\rho\rho^3$. Therefore one gets a potential

$$V(\rho_x) = -C\rho_x + \rho_x^2 + \lambda(\rho_x^2 - 1)^2 - 3log(\rho_x), \tag{10}$$

where

$$C = \kappa \mathrm{Tr}(\sum_\mu \rho_{x+\mu} \alpha_x^\dagger U_{x,\mu} \alpha_{x+\mu}) \quad . \tag{11}$$

We have plotted this local $V(\rho)$ potential in fig. 1. for $\lambda = 0.0001$ and for a typical $C = 2$ value. The potential has one minimum, but is not symmetric with respect to its minimum. By a simple analysis of $V(\rho)$ one can show, that it has only one minimum for $\lambda < (3/2 + \sqrt{11}/2)^2 \approx 9.98$. For even larger values of λ, one needs $\kappa \approx \mathcal{O}(10)$ to have a second minimum. These κ-s are clearly out of any range of physical interest. Thus, we can assume that $V(\rho)$ has only one minimum.

The procedure to perform the overrelaxation step in ρ is now clear. For each ρ_x calculate the value of $\rho_x^{'} \neq \rho_x$ such that $V(\rho_x) = V(\rho_x^{'})$. Note that this is not just a reflection with respect to the minimum of the potential as $V(\rho)$ is not symmetric. In practice we found that a reliable way to determine $\rho^{'}$ is to calculate the first, second and third derivatives of V (analytically) and calculate $\rho_x^{'}$ for which the Taylor polynom gives the same value for the potential. After this starting step one-two Newton iterations give the proper $\rho_x^{'}$ value with a relative accuracy of 10^{-6}. If the first step can not be made, or turns out to be too rude Newton alone or bisection can be used.

The non-trivial part of the overrelaxation step in ρ is the observation that $\rho^{'}$ is a nonlinear function of ρ. Therefore, the transformation of ρ to $\rho^{'}$ does not leave the measure invariant.

As a consequence, one has to correct for this by a reject/accept step. In order to obtain the proper updating procedure let us consider the stability equation for ρ.

$$\int d\rho T(\rho,\bar{\rho})P(\rho) = P(\bar{\rho}), \tag{12}$$

where $P(\rho)$ is the equilibrium distribution in ρ and $T(\rho,\bar{\rho})$ is the overrelaxation operator. It has the form

$$\int_a^b d\rho T(\rho,\bar{\rho}) = \begin{cases} 0 & \text{if} \quad M(\bar{\rho}) \notin (a,b) \\ A(\bar{\rho}) & \text{if} \quad M(\bar{\rho}) \in (a,b) \end{cases} \tag{13}$$

where $M(\rho)$ is the "mirror image" of ρ, thus

$$V(M(\rho)) = V(\rho) \qquad , \qquad \text{but} \qquad \rho \neq M(\rho), \tag{14}$$

unless ρ is exactly at the minimum, where $\rho = M(\rho)$, of course. Evaluating the above stability integral on gets

$$\int d\rho A(\bar{\rho})\delta(\rho - M(\bar{\rho}))P(\rho) = A(\bar{\rho})\frac{1}{|dM(\bar{\rho})/d\bar{\rho}|}P(\bar{\rho}). \tag{15}$$

Combining this with the stability equation one obtains

$$A(\rho) = |M^{'}(\rho)| = |\frac{d\rho^{'}}{d\rho}| = |\frac{dV}{d\rho}/\frac{dV}{d\rho^{'}}| \quad . \tag{16}$$

The Monte-Carlo realization of the above $T(\rho,\rho^{'})$ overrelaxation operator can be done in the following way. One determines $M(\rho)$ "mirror image" of ρ and calculates the $V^{'}(\rho)$ and $V^{'}(M(\rho))$ derivatives. The $\rho \to M(\rho)$ updating is accepted if

$$|\frac{V^{'}(\rho)}{V^{'}(M(\rho))}| > r, \tag{17}$$

where r is a random number between 0 and 1. Otherwise the updating is rejected. In practice we found the acceptance always to be larger than 80%.

Note, that the same result can be obtained by considering the probability densities. The probability of finding the system in a state with local energy between V and $V + \Delta V$ is a sum of two probabilities. The probability to find it between ρ and $\rho + \Delta\rho$ plus the probability to find it between $M(\rho)$ and $M(\rho) + \Delta M(\rho)$, where $V(\rho) = V(M(\rho)) = V$ and $V(\rho + \Delta\rho) = V(M(\rho) + \Delta M(\rho)) = V + \Delta V$. Since we want the algorithm to be microcanonical, $dV = V^{'}(\rho)d\rho - V^{'}(\rho^{'})d\rho^{'} = 0$ ($\rho^{'} = M(\rho)$). Clearly one regains (16) for $A(\rho)$ and the reject/accept step (17).

3

We have tested the algorithm described above in the SU(2)-Higgs model. For parameter values $\lambda = 0.0001$, $\beta = 8$ and $\kappa = 0.129$ the system is in the Higgs region of the model. We measured the normalized autocorrelation function Γ_O of some operator O which is defined as

$$\Gamma_O(t) = \frac{< O(0)O(t) > - < O(0) >^2}{< O(0) >^2} \tag{18}$$

where t indicates a fictitious Monte Carlo time corresponding to the number of sweeps. Γ_O falls off exponentially

$$\Gamma_O(t) \propto \exp(-t/\tau) \ \text{ for } \ t \to \infty \tag{19}$$

which defines the exponential autocorrelation time τ. In fig.2 we plot the autocorrelation function Γ_ρ for the length of the Higgs field ρ. This operator in general shows the longest autocorrelation time in the SU(2)-Higgs model. The solid line corresponds to a pure Metropolis simulation and the dashed line shows the result of a hybrid overrelaxation with a mixing ratio of Metropolis to overrelaxation 1:1. The measurements have been performed after each sweep of a Metropolis or an overrelaxation update through the lattice. Although the lattice used is quite small (8^4) the autocorrelation function for the Metropolis algorithm shows a very slow fall off, indicating an autocorrelation time of about $\tau_{Met} \approx 130$. On the other hand the hybrid overrelaxation algorithm gives a considerable improvement, $\tau_{OR} \approx 25$, over the Metropolis algorithm [2]. The results for the exponential autocorrelation times τ eq.(19), given above, have been checked against the integrated autocorrelation times and a complete agreement has been found.

The dashed curve in fig.2 corresponds to a combination of only one Metropolis to one overrelaxation step. We want to note that the main effect of the improvement stems from the overrelaxation in ρ alone. Switching off the overrelaxation in U and α we found an almost identical autocorrelation function. This clearly demonstrates that the operator ρ gives the slowest mode. Increasing the mixing ratio of Metropolis to overrelaxation steps does not improve the autocorrelation time. This is understandable from the ρ-potential eq.(10) as more overrelaxation steps reflects ρ only back and forth, not leading to substantial changes in the configuration.

4

In simulations of the SU(2)-Higgs model, which is the most relevant part for studies of the electroweak phase transition, using a Metropolis algorithm one detects large autocorrelation

[2] Based on the ideas of the present letter, a hybrid of heatbath and overrelaxation was analyzed in [8] and a similar improvement was found.

times already on small lattices. In order to be able to have reliable numerical results it is therefore necessary to find an algorithm which improves this behaviour. We have extended the overrelaxation algorithm which seems to work very efficient in pure gauge theories to the SU(2)-Higgs model. The treatment of the radial part of the Higgs-field in the algorithm led to an additional accept/reject step which corrects for the measure term.

We have tested our version of the overrelaxation algorithm in the SU(2)-Higgs model at parameter values interesting for comparisons with perturbation theory. As fig.2 shows, the autocorrelation time can be reduced substantially, namely from $\tau \approx 130$ in the Metropolis algorithm (solid line) to $\tau \approx 25$ in the overrelaxation algorithm. We want to emphasize that this result is obtained on a small (8^4) lattice. It is expected that the hybrid overrelaxation algorithm has a dynamical critical exponent of $z \approx 1$ as compared to the Metropolis or heatbath with $z \approx 2$. Therefore one can expect even better improvements on larger lattices.

We found it sufficient to perform only one overrelaxation step in the length of the Higgs field ρ to obtain the best improvement. We expect, however, that as in pure gauge theories [6, 3], one can obtain even smaller autocorrelation times by tuning the mixing ratio of Metropolis to overrelaxation steps for the update of the gauge field U and the angle of the Higgs field α. This tuning will depend on the parameter values where simulations are performed. The optimal mixing ratio should be determined from case to case.

We think that our numerical results are very promising and that the hybrid overrelaxation we are suggesting is a big improvement over algorithms used so far for simulations of the SU(2)-Higgs model. We hope that by careful fine tuning of the mixing ratio of different algorithms for the update of the variables U, ρ and α the autocorrelation times might be reduced to small numbers $\tau < 10$ as it can be obtained in pure gauge theories and one can therefore obtain high precision numerical data to shed new light on the the electroweak phase transition beyond perturbation theory.

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Figure Caption

Fig.1 The local potential eq.(10) as a function of the radial length of the scalar field ρ for $\lambda = 0.0001$ and $C = 2$.

Fig.2 The logarithm of the autocorrelation function for the length of the Higgs field ρ as a

function of the Monte Carlo "time" t. The parameter values are $\beta = 8$, $\lambda = 0.0001$ and $\kappa = 0.129$ and belong to a point in the Higgs region of the model. The lattice is 8^4. The solid line is the Metropolis algorithm alone. The dashed line is a hybrid of one Metropolis to one overrelaxation step.

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