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Playing with the kinetic term in the HMC

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The HMC algorithm, combining the advantages of molecular dynamics and Monte-Carlo methods, is the most efficient algorithm to simulate QCD including the effects of sea quarks. In the standard approach momentum fields are generated with a Gaussian probability density. In this work I will explore another possibility. By using a Lorentz distribution one can dynamically impose a cutoff in the rate of change of the coordinates that potentially could have a better behavior. I will present some results in pure $SU(2)$ gauge theory.

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1. Introduction

In a QCD lattice simulation the fermionic degrees of freedom are integrated out, producing a non local effective gauge action that increases dramatically the cost of evaluating any update. Algorithms based on local updates are terribly inefficient in simulating these kinds of systems. The Hybrid Monte Carlo (HMC) algorithm [1] combines a molecular dynamics update scheme with a Metropolis-Hastings accept-reject step to produce global update proposals but keeping a high acceptance probability. These unique characteristics make the HMC algorithm the only choice for large-scale QCD simulations.

The global update proposals of the HMC come from a Hamiltonian flow

$$H(p,q) = \frac{p^2}{2} + S[q], \tag{1.1}$$

where we represent by q the fields of the system that we want to study and by p the additional conjugate momenta variables. These additional conjugate momenta follow a gaussian probability distribution. In physical systems this kinetic term is a consequence of Galilean and rotational invariance. But these are symmetries that we do not have to obey in our lattice simulations. We can choose different kinetic terms if they produce a more effective sampling.

In this work we are going to analyze two different ways to explore phase space by changing the kinetic term. The standard kinetic term produces via the equation of motion $\dot{q} = \frac{\partial H}{\partial p} = p$ a rate of change of the variables that also follows a Gaussian distribution. In our update process the change in the values of the coordinates is therefore centered at zero with a few variables changing by a large amount. As an alternative we are going to use the Hamiltonian

$$H(p,q) = \log\left(1 + \frac{p^2}{2\gamma^2}\right) + S[q] \tag{1.2}$$

making our momenta follow a Lorentz distribution $\propto \frac{1}{1+p^2/2\gamma^2}$. These conjugate momenta are also centered around zero, but their fluctuations don't have a typical scale. This may seem a bad idea because very large momenta will kick the variables away, thus making our numerical integration of the equations of motion difficult. But the situation is just the opposite. The equation of motion for our variables reads now

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{2p}{\gamma^2 + p^2} \tag{1.3}$$

and therefore this kinetic term effectively imposes a dynamic cutoff in the rate of change of our variables: $\dot{q}$ can not be bigger than $1/\gamma$. Very large momenta or forces are not dangerous in the modified algorithm because they simply "freeze" the conjugate link variables instead of kicking them. Moreover, the distribution of $\dot{q}$ peaks close to its maximum possible value. In this way we produce a motion in phase space that is on average faster by avoiding very large updates.

We are going to compare the standard HMC algorithm and the modified one with a Lorentz kinetic term (we will call it HMCL) in a pure $SU(2)$ gauge theory.

2. Implementation in pure $SU(2)$ gauge theory

We are going to consider pure $SU(2)$ gauge theory (the extension to other gauge groups is straightforward). The links $U_\mu(x) \in SU(2)$ take values in the group, and elements of the algebra

$\pi \in \mathfrak{su}(2)$ can be written as

$$\pi = \sum_{a=1}^{3} \pi^a T^a \tag{2.1}$$

where T^a are the $SU(2)$ generators (the $T^a = \sigma^a/2$ with σ^a being the Pauli matrices).

We are going to study the plaquette action

$$S[U] = \frac{\beta}{2} \sum_p Tr(1 - U_p), \tag{2.2}$$

where U_p is the product of the links in a simple plaquette and the sum is over all oriented plaquettes. For each link $U_\mu(x) \in SU(2)$ we introduce an algebra-valued conjugate momenta $\pi_\mu(x) \in \mathfrak{su}(2)$. The Hamiltonian that defines the standard HMC algorithms is given by

$$H(\pi, U) = \sum_{x,\mu,a} \frac{\left[\pi^a_\mu(x)\right]^2}{2} + \frac{\beta}{2} \sum_p Tr(1 - U_p) \tag{2.3}$$

with equations of motion

$$\dot{\pi}^a_\mu(x) = -\frac{\partial H(\pi, U)}{\partial U_\mu(x)} = -\frac{\beta}{4} Tr\left[T^a U_\mu(x) \sum_{\nu \neq \mu} M_{\mu\nu}(x) \right] \tag{2.4}$$

$$\dot{U}_\mu(x) = \frac{\partial H(\pi, U)}{\partial \pi_\mu(x)} = \pi_\mu(x) U_\mu(x) \tag{2.5}$$

where $M_{\mu\nu}(x)$ are the sum of "staples" of Wilson lines from x to $x + \mu$. The Hamiltonian of the modified (HMCL) algorithm is given by[1]

$$H_L(\pi, U) = \sum_{x,\mu,a} \log\left[1 + \left(\pi^a_\mu(x)/\gamma\right)^2\right] + \frac{\beta}{2} \sum_p Tr(1 - U_p). \tag{2.6}$$

Only the equation of motion for $U_\mu(x)$ is modified, that now reads

$$\dot{U}_\mu(x) = \frac{\partial H(\pi, U)}{\partial \pi_\mu(x)} = \sum_a \left[\frac{2\pi^a_\mu(x)}{\gamma^2 + (\pi^a_\mu(x))^2} T^a \right] U_\mu(x) \tag{2.7}$$

while the equation of motion for the momenta (the computation of the forces) remains unchanged.

Together with the change in the equation of motion of $U_\mu(x)$ we need two additional changes to our standard HMC algorithm in order to achieve the desired equilibrium properties. First the momentum refresh has to be done using a Lorentz distribution[2] with scale γ. Second, one has to accept the update with a probability $\min(1, e^{-\Delta H_L})$ where H_L is given by equation (2.6).

[1] Note that the sum in the internal "color" index a is *outside* the log.

[2] Generating random samples of this distribution is straightforward, since this probability density function is easily integrable.

2.1 Details of the simulations and observables

We simulate at three different values of the coupling $\beta = 2.4, 2.5, 2.6$ that should span roughly a factor two change in the scale ($a \sim 0.06 - 0.12$ fm), and two volumes $V = 12^4, 16^4$. The molecular dynamics equations of motion are integrated using the Omelyan integrator [2] with the standard value of $\lambda = 0.185$.

The HMCL algorithm has an extra parameter γ to tune. This parameter can be interpreted as a rescaling in the molecular dynamics time and in this sense is similar to a mass term in the normal HMC algorithm. Obviously the smaller this mass parameter is, the faster one will move trough phase space, but this has a cost in terms of acceptance ratio. Here we will tune the γ parameter to achieve similar acceptance ratios on both the HMC and the HMCL setups. This is achieved with $\gamma = 0.8$.

We will measure Wilson loops of sizes 1×1 (the plaquette), and also 2×2 and 4×4. We will also look at the topological charge. We use the clover definition of $F_{\mu\nu}$ to compute

$$Q = \frac{1}{32\pi^2} \sum_x \varepsilon_{\mu\nu\rho\sigma} F_{\mu\nu}(x) F_{\rho\sigma}(x). \tag{2.8}$$

It is well known that Monte-Carlo configurations contain large UV fluctuations that hide large-scale structures like the topological charge. We will apply a smoothing process to our gauge configurations, in particular an under relaxed cool [3]

$$U_\mu^{(n+1)}(x) \longrightarrow \mathscr{P}\{\alpha U_\mu^{(n)}(x) + \sum_\nu M_{\mu\nu}(x)\} \tag{2.9}$$

in which each link is averaged with its six "staples" and then projected back to the group. We apply 60 steps with $\alpha = 2$.

3. Results

Both the HMC and the HMCL algorithm allow us to measure observables in a sample of the equilibrium distribution $\{O_\alpha(t); t = 1, \ldots, N\}$ (the index $\alpha = 1, \ldots, N_{\text{obs}}$ labels the observables). These measurements are statistically correlated, and the autocorrelation function quantifies these correlations

$$\Gamma_\alpha(t) = \frac{1}{N} \sum_{t=1}^{N} \left(O_\alpha(t) - \overline{O}_\alpha\right) \left(O_\alpha(0) - \overline{O}_\alpha\right)\rangle, \tag{3.1}$$

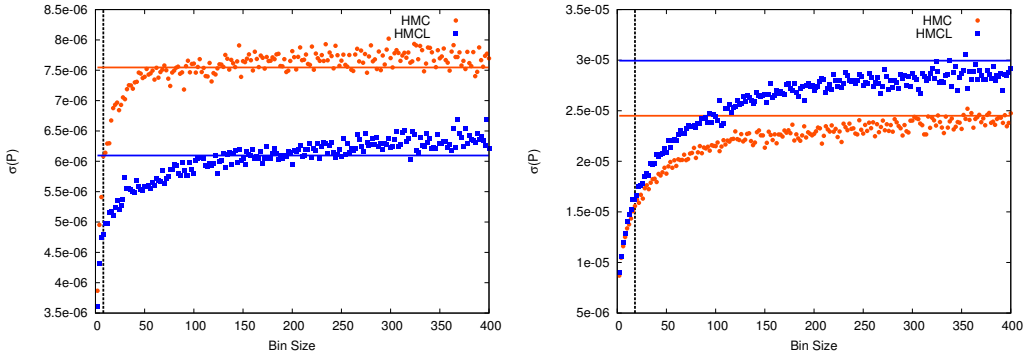
where $\overline{O}_\alpha$ is the statistical mean of the observable α.

These correlations have to be taken into account when computing the statistical error of an observable (see for example [4]). In our case it is given by

$$\sigma_\alpha = \sqrt{\frac{2 v_\alpha \tau_{\text{int},\alpha}}{N}} \tag{3.2}$$

where v_α is the variance of the observable α (that is, $\Gamma_\alpha(0)$), and $\tau_{\text{int},\alpha}$ is the integrated autocorrelation time of the observable, defined as

$$\tau_{\text{int},\alpha} = \frac{1}{2} + \frac{1}{v_\alpha} \sum_{t=1}^{\infty} \Gamma_\alpha(t). \tag{3.3}$$



(a) Plaquette (b) $\langle W_{4\times4}\rangle$

Figure 1: Error versus the bin size. The vertical dashed line represents $2\tau_{\rm int}$ and is plotted for reference only. The horizontal lines corresponds to the error computed by computing $\tau_{\rm int}$ (see text for more details).

	$V = 12^4$			$V = 16^4$		
$\langle\ldots\rangle$	$\beta = 2.4$	$\beta = 2.5$	$\beta = 2.6$	$\beta = 2.4$	$\beta = 2.5$	$\beta = 2.6$
$W_{1\times1}$	1.259998(11)	1.3040202(99)	1.3401848(77)	1.259995(16)	1.303919(13)	1.340050(12)
	1.260004(11)	1.3040278(93)	1.3401944(62)	1.259982(15)	1.303952(11)	1.3400554(94)
$W_{2\times2}$	0.444850(25)	0.516329(25)	0.575913(19)	0.444825(36)	0.515973(31)	0.575331(32)
	0.444865(30)	0.516315(30)	0.575928(20)	0.444790(40)	0.516035(32)	0.575352(38)
$W_{4\times4}$	0.026182(12)	0.048300(25)	0.072296(21)	0.026167(17)	0.048031(25)	0.071383(41)
	0.026194(16)	0.048362(29)	0.072288(26)	0.026157(20)	0.048061(30)	0.071385(57)
Q^2	2.650(12)	0.8523(87)	0.1232(40)	8.451(83)	3.055(56)	0.808(36)
	2.661(16)	0.849(12)	0.1266(51)	8.48(11)	3.068(78)	0.786(46)

Table 1: Observables measured in the run with their uncertainties. The first line are results of the standard HMC algorithm, whereas the second line corresponds to the results of the HMCL algorithm. As one can see, the agreement between both algorithms is almost perfect.

One can proceed through the previous formulas to compute the uncertainties of the observables, or one can use the popular alternative of binning methods, in which data is averaged over sections of the Monte Carlo history of large enough length so that these measurements can be considered independent. In our particular case, with very long Monte Carlo histories both methods are straightforward to apply and give the same results (see figure 1), but when this is not the case the discussion is more subtle [5].

Since in our setup both algorithms need the same computing time to produce an additional member of the Markov chain, and the acceptance probabilities in both algorithms are similar, the question of which algorithm performs better is answered by looking at the algorithm that "decorrelates" faster, producing smaller uncertainties. Table 1 summarizes the results for different observables.

One observe that the results are very similar between the two algorithms, with a difference in the uncertainties in the range $\pm30\%$, and this difference seem to be constant for all values of β and the volume (i.e. neither algorithm seems to have a better *scaling* than the other). Nevertheless

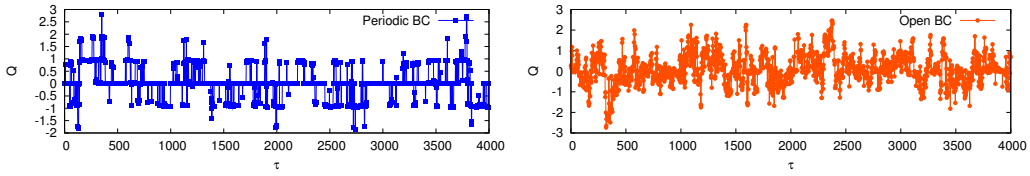


Figure 2: Sample of the Monte Carlo history of the topological charge with open and periodic boundary conditions for the volume $V = 12^4$ and $\beta = 2.5$.

	$V = 12^4$			$V = 16^4$		
$\langle \ldots \rangle$	$\beta = 2.4$	$\beta = 2.5$	$\beta = 2.6$	$\beta = 2.4$	$\beta = 2.5$	$\beta = 2.6$
$W_{1\times 1}$	1.190795(20)	1.235107(17)	1.273033(16)	1.207584(26)	1.251767(20)	1.28924(16)
	1.190795(19)	1.235084(17)	1.27298(13)	1.207604(22)	1.251780(19)	1.28924(15)
$W_{2\times 2}$	0.363959(38)	0.425108(35)	0.478480(30)	0.383586(53)	0.447091(42)	0.501832(33)
	0.363959(44)	0.425084(41)	0.478392(34)	0.383622(57)	0.447093(49)	0.501830(41)
$W_{4\times 4}$	0.015822(16)	0.029544(23)	0.045165(25)	0.018301(22)	0.034012(31)	0.051318(29)
	0.015826(19)	0.029555(27)	0.045103(34)	0.018362(26)	0.033976(37)	0.051365(39)
Q^2	1.334(11)	0.4849(71)	0.1409(39)	5.398(96)	1.840(41)	0.599(27)
	1.336(14)	0.4850(90)	0.1453(68)	5.25(10)	1.933(57)	0.598(34)

Table 2: Observables measured in the runs with open boundary conditions. The first line are results of the standard HMC algorithm, whereas the second line corresponds to the results of the HMCL algorithm. These results draw the same conclusions as the runs with periodic boundary conditions.

all observables but the plaquette decorrelate faster with the standard kinetic term of the HMC algorithm than with the modified version.

The biggest difference is found in the topological susceptibility. It is known that simulations suffer from a critical slowing down when approaching the continuum limit, and that this problem is more severe for topological quantities [5] and recently the solution of simulating with open boundary conditions have been proposed [6]. We wanted to see if the previous conclusions remain unchanged when simulating with open boundary conditions.

3.1 Simulations with open boundary conditions

By using open (Neumann) boundary conditions in the time direction the topological charge can go in and out the lattice. This has the effect observed in the histories of Fig. 2, where by simple observations one can see that the measurements of the topological charge are less correlated in the runs with open boundary conditions.

Nevertheless, as the results of the Table 2 show, the conclusions remain unchanged for the runs performed with open boundary conditions: There is not much difference between both algorithms, and only the plaquette decorrelates faster with the HMCL algorithm.

4. Conclusions

By changing the kinetic term in the Hybrid Monte Carlo we have investigated another way to explore the phase space. The equations of motion of the modified Hamiltonian impose dynamically

a cutoff in the rate of change of the coordinates, avoiding the effects of either large forces or momenta. In this way we pretend a faster exploration of phase space. This modification does not need any change in the evaluation of the molecular dynamics forces, and is thus easy to implement over an existing HMC simulation code.

We have compared the standard and modified kinetic terms in pure $SU(2)$ gauge theory by generating long Markov chains at two different volumes, three values of the coupling and different boundary conditions (periodic and open). By tuning both algorithms to use the same computer time per trajectory, and to have the same acceptance ratio, a meaningful comparison between both algorithms can be done by simply looking at which algorithm decorrelates faster the measurements, that would translate in smaller uncertainties at the same computational cost. We have investigated different observables: Wilson loops of different sizes and the topological susceptibility.

We find that both algorithms perform rather similarly, with a difference in the uncertainties of around $\pm 30\%$ for all values of the coupling or of the volume (that is: both algorithms have a similar scaling). It seems that the modified kinetic term tends to decorrelate faster the plaquette (a very local observable), while larger Wilson loops or the topological susceptibility tends to decorrelate faster with the standard kinetic term.

Having very similar performances, and noting that usually one is interested in quantities less local than the plaquette, there seems to be no advantage, but a worsening in performance, in the use of the modified kinetic term in terms of producing "more independent" samples of the equilibrium distribution.

Still, it is not in the pure gauge theory where the effect of large forces is problematic, rather in the simulation of dynamical fermions. These simulations can benefit from having a cutoff in the rate of change of the coordinates. This point needs further investigations.

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References

[1] S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, *Phys. Lett.* **B195** (1987) 216–222.

[2] I. Omelyan, I. Mryglod, and R. Folk, *Comput. Phys. Commun.* **151** (2003) 272–314.

[3] C. Michael and P. Spencer, *Phys.Rev.* **D50** (1994) 7570–7577, [hep-lat/9404001].

[4] **ALPHA collaboration** Collaboration, U. Wolff, *Comput.Phys.Commun.* **156** (2004) 143–153, [hep-lat/0306017].

[5] **ALPHA** Collaboration, S. Schaefer, R. Sommer, and F. Virotta, *Nucl. Phys.* **B845** (2011) 93–119, [arXiv:1009.5228].

[6] M. Luscher and S. Schaefer, *JHEP* **1107** (2011) 036, [arXiv:1105.4749].