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Cooling of SU(3) Lattice Gauge Field Configurations

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Abstract

A method to cool SU(3) lattice gauge field configurations is discussed. It locally minimizes the mean plaquette. The cooled configurations can be used to compute the η' -mass in QCD, using Witten's formula connecting this mass to the topological susceptibility.

1. Introduction and motivation

One of the longstanding problems in high energy physics is the so-called U(1) problem [1-3]: why is the mass of the particle associated with the axial singlet current not small, as expected for a Goldstone particle. By now the qualitative solution to this problem is well-established [4], namely instantons generate an effective mass-term for the η' and so the classical chiral symmetry is broken at the quantum level. Moreover, there exists a quantitative handle on the problem now, due to a connection between the η' -mass and the topological susceptibility χ_t [5,6] in the pure gauge theory, a quantity that is measurable in Monte Carlo simulations of lattice gauge theory. With the conventions of [1] the expression for the topological susceptibility is

$$\chi_t = \frac{1}{(32\pi^2)^2} \int d^4x \langle \tilde{F}\tilde{F}(x) \tilde{F}\tilde{F}(0) \rangle, \quad (1.1)$$

where $\tilde{F}\tilde{F}(x) = F_{\mu\nu}^a(x) \frac{1}{2} \epsilon_{\mu\nu\kappa\lambda} F_{\kappa\lambda}^a(x)$, and $\langle \rangle$ indicates the path integral average over all gauge field configurations.

Up to now various authors have measured topological susceptibility in 2 and 4 dimensional models [7-13], by measuring the topological charge directly in a number of configurations. We want to exploit the property that, in the continuum, sectors of the theory with different topological charge are disconnected, and the minimum action for SU(N) gauge theory in a sector with charge n equals [14]

$$|n| \star \frac{4\pi^2}{N}. \quad (1.2)$$

Note that as usual in lattice gauge theory [15] we have taken an explicit factor $\beta = \frac{2N}{g^2}$ out of the action, so that the path integral measure becomes $e^{-\beta S}$ and

$$S = \frac{1}{8N} \int d^4x F_{\mu\nu}^a F_{\mu\nu}^a \quad (1.3)$$

is called the action.

If one is able to cool configurations without losing the topological charge, the action of the configuration converges to the minimum action in that sector and one is able to read off the charge of the configuration from the action value. The feasibility of such a program on the lattice was shown in early calculations in the 2 dimensional $O(3)$ sigma model [9], where it was found that the action drops quickly to a minimum value which is maintained during many subsequent cooling sweeps. After many sweeps the topological charge may change and a further steep drop sets in; however the minimum value is easily recognizable. This was also observed in 4-dimensional $SU(2)$ gauge theory [11], though with the standard Wilson action the configurations tended to lose their charge quickly. The cooling scheme we want to utilize calculates for each link in turn the $SU(3)$ matrix that minimizes the action of the configuration, keeping the matrices on all the other links fixed. The action for $SU(N)$ pure gauge theory is [16]:

$$\sum_{x, \mu, \nu \neq \mu} \left(1 - \frac{1}{N} \operatorname{Re} \operatorname{Tr} (U_{x, \mu} U_{x+a_\mu, \nu} U_{x+a_\nu, \mu}^+ U_{x, \nu}^+)\right), \quad (1.4)$$

where x denotes the lattice sites, μ and ν are directions and a_μ is a unit vector in the μ -direction. Thus the procedure is to calculate for a fixed link (x, μ) the total "force"

$$F_{x\mu} = \sum_{\nu \neq \mu} (U_{x+a_\mu, \nu} U_{x+a_\nu, \mu}^+ U_{x, \nu}^+ + U_{x-a_\nu, \mu}^+ U_{x-a_\nu, \mu} U_{x-a_\mu, \nu}) \quad (1.5)$$

on it and then determine the $SU(N)$ matrix $V_{x\mu}$ that maximizes

$$\operatorname{Re} \operatorname{Tr} (F_{x\mu} V_{x\mu}). \quad (1.6)$$

Finally the matrix $U_{x\mu}$ is replaced by $V_{x\mu}$. For $SU(2)$ this procedure is trivial, as a sum of products of $SU(2)$ matrices is a $SU(2)$ matrix again when divided by its determinant. For $SU(3)$ the problem is quite complicated and will be discussed in section 2. In section 3 the implementation of the algorithm of section 2 is discussed and section 4 contains some examples and general discussion.

2. Cooling of a link.

The problem, as stated in the introduction, is to find a $SU(N)$ matrix V maximizing

$$\operatorname{Re} \operatorname{Tr} (F V), \quad (2.1)$$

given a force F on the link. In order to find V we first make a polar decomposition of F ,

$$F = H U_1 e^{i\sigma}, \quad (2.2a)$$

$$H = (FF^+)^{\frac{1}{2}}, \quad (2.2b)$$

where $U_1 \in SU(N)$ and the phase σ can be restricted to the range

$$\sigma \in \left(-\frac{\pi}{N}, \frac{\pi}{N} \right] \quad (2.2c)$$

as the centre of $SU(N)$ is Z_N . As H is hermitean it can be diagonalized with a $SU(N)$ - matrix U_2 ,

$$H = U_2^+ D U_2, \quad D = \text{diag} (d_i), \quad (2.3a)$$

where, because H is positive semi-definite,

$$d_i \in \mathbb{R}^+. \quad (2.3b)$$

So the problem can be restated as: find the $SU(N)$ - matrix

$$U = U_2 U_1 V U_2^+ \quad (2.4)$$

that maximizes

$$f_1 \equiv \text{Re Tr} (U D e^{i\sigma}) \quad (2.5)$$

By choosing U_2 appropriately we can arrange for the d_i to be ordered:

$$d_1 > d_2 > d_3 \quad (2.6)$$

and since an overall factor in D factors out in (2.5) either all d 's are zero or effectively

$$d_1 = 1, \quad 0 < d_3 < d_2 < 1. \quad (2.7)$$

In case all d 's vanish, the force F on the link (x, μ) vanishes and the link variable will be left unchanged. In practice it was also done if all the d_i were $< 10^{-3}$, but this never occurred in 10^8 updates. From now on we will assume (2.7).

For $N=2$ finding the solution of (2.5) is trivial. We now specialize to $N=3$ and use the parametrization

$$U = (v \quad w \quad v^* \wedge w^*) \quad (2.8)$$

where v and w are complex vectors subject to the constraints

$$v \cdot v^* = w \cdot w^* = 1, \quad v \cdot w^* = 0. \quad (2.9)$$

The easier way to impose these constraints with Lagrange multipliers is to regard complex numbers and their conjugates as independent variables and maximize

$$\begin{aligned} \text{Re Tr } (U D e^{i\sigma}) - \lambda_1 (\|v\|^2 - 1) - \lambda_2 (\|w\|^2 - 1) \\ - \lambda_3 (w, v) - \lambda_4 (w, v)^* \end{aligned} \quad (2.10)$$

The same results can be obtained with considerably more effort by maximizing

$$\begin{aligned} \text{Re Tr } (U D e^{i\sigma}) - \frac{1}{2} \mu_1 (\|v\|^2 - 1) - \frac{1}{2} \mu_2 (\|w\|^2 - 1) \\ - \mu_3 \text{Re } (v, w) - \mu_4 \text{Im}(v, w) \end{aligned} \quad (2.11)$$

The generic solution of maximizing (2.5) is that U must be diagonal. In case $d_3=0$ there are many solutions, among which is a diagonal one. In practice this case was avoided by not updating the link-variable if $d_3 < 10^{-3}$, but this never occurred in 10^8 updates. So from now on we will assume

$$d_3 > 0. \quad (2.12)$$

Trying to solve the equations for the diagonal elements of U leads to an eighth-order equation. Therefore we reparametrize U first as

$$U = \text{diag } (e^{i\phi}, e^{i\psi}, e^{-i(\phi+\psi)}) , \quad (2.13)$$

whereby

$$f_2 \equiv f_1 / d_1 \quad (2.14)$$

takes the form

$$f_2 = \cos(\phi+\sigma) + d_2 \cos(\phi+\sigma) + d_3 \cos(\sigma-\phi-\psi). \quad (2.15)$$

By the same argument leading to (2.2c) we may assume

$$\phi \in \left[-\frac{\pi}{3}, \frac{\pi}{3}\right]. \quad (2.16)$$

Solving $\partial f_2 / \partial \phi = 0$ and introducing

$$\tau = \tan(\sigma/2) \in \left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right], \quad (2.17a)$$

and

$$t = \tan(\phi/2) \in \left[-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right] \quad (2.17b)$$

the problem reduces to a maximalisation problem in one parameter,

$$f_3 = \left\{1 + \frac{2d_3}{1+d_3^2} (t_1\tau_1 + t_2\tau_2)\right\}^{\frac{1}{2}} + \frac{d_2}{\sqrt{1+d_3^2}} (t_1\tau_3 + t_2\tau_4), \quad (2.18a)$$

$$f_3 \equiv f_2 \sqrt{1+d_3^2}, \quad (2.18b)$$

$$t_1 = (1-t^2)/(1+t^2), \quad t_2 = 2t/(1+t^2), \quad (2.18c)$$

$$\tau_1 = ((1-\tau^2)^2 - 4\tau^2)/(1+\tau^2)^2, \quad \tau_2 = 4\tau(1-\tau^2)/(1+\tau^2)^2, \quad (2.18d)$$

$$\tau_3 = (1-\tau^2)/(1+\tau^2), \quad \tau_4 = -2\tau/(1+\tau^2). \quad (2.18e)$$

Note that for $\tau = 0$ the solution is $t_{\max} = 0$ and because of the invariance of f_3 under $\tau \rightarrow -\tau$ and $t \rightarrow -t$ only the sector $\tau \in [0, 1/\sqrt{3}]$ needs to be investigated. The solution of maximizing f_3 is not analytical. To demonstrate that the problem will be analyzed for $\tau = 1/\sqrt{3}$. For this τ -value τ_1/τ_2 equals τ_3/τ_4 , so f_3 reduces to

$$f_4 \equiv f_3(\tau=1/\sqrt{3}) = \left\{1 + \frac{2d_3}{1+d_3^2} x\right\}^{\frac{1}{2}} - \frac{d_2}{\sqrt{1+d_3^2}} x, \quad (2.19a)$$

$$x = (t^2 + 2t\sqrt{3} - 1)/(2(t^2+1)). \quad (2.19b)$$

The solution separates the (d_2, d_3) - plane in 2 sections divided by the

line

$$d_3 = d_{3s} \equiv d_2/(1+d_2) . \quad (2.20)$$

In region I, where $d_3 < d_{3s}$, $\partial x/\partial t=0$ leads to the maximum and $t_{\max} = -1/\sqrt{3}$.

In region II ($d_3 > d_{3s}$) the maximum is obtained for

$$x = x_0 \equiv d_3/2d_2^2 - (1+d_3^2)/2d_3 , \quad (2.21a)$$

where $f'(x_0) = 0$. The relevant root is

$$t_{\max} = \{2\sqrt{1-x_0^2} - \sqrt{3}\}/(1-2x_0) . \quad (2.21b)$$

In region I all derivatives of $t_{\max}$ vanish and in region II the derivatives are regular away from $d_3=d_{3s}$, where they diverge:

$$\left. \frac{\partial t_{\max}}{\partial \tau} \right|_{II} \left(\tau = \frac{1}{\sqrt{3}} \right) = ((2-d_2)d_3+d_2)/((1+d_2)d_3-d_2) , \quad (2.22a)$$

$$\left. \frac{\partial t_{\max}}{\partial x_0} \right|_{II} \left(\tau = \frac{1}{\sqrt{3}} , d_3=d_{3s} + \epsilon \right) = \epsilon^{-\frac{1}{2}}(d_2 d_{3s})^{\frac{1}{2}} \left(\frac{1}{3} \sqrt{2} - \frac{1}{9} \sqrt{3} \right) + O(\epsilon^{\frac{1}{2}}) \quad (2.22b)$$

($\partial x_0/\partial d_2$ and $\partial x_0/\partial d_3$ are regular and non-zero).

As the solution is not known in closed form and is non-analytical, the maximizing of the function f_3 is left as a numerical maximization. This is described in the next section.*

3. Implementation

Most of the algorithms involved in implementing the steps described in the previous section are standard, though special routines have been written for all of them in order to speed up the execution. On the Atlas-10 (Fujitsu M380) which has 32-bit arithmetic it is necessary to do the majority of the calculations in double precision.

The numerical maximization of f_3 (2.18) is done by finding a starting value from a table as described below and then maximizing by parabolic

* During the drafting of this paper we were informed that a method similar to that described above was used in Monte Carlo renormalization group studies in [18].

interpolation and uphill search [17]. Typical distributions of $|\tau|$ (2.17a) and d_2, d_3 (2.3a, 2.7) are shown in figures 1 and 2. During the cooling $|\tau|$ will diminish and d_2 and d_3 tend to 1. The look-up table contains the value of $t_{\max}$ for 10 equally spaced points in the intervals $[10^{-3}, 1]$ for d_2 , $[10^{-3}, d_2]$ for d_3 and $n_\tau=21$ points in the interval $[0, 1/\sqrt{3} - 10^{-3} = \tau_{\max}]$ spaced logarithmically:

$$\tau_j = \log(j/b+1), \quad b=(n_\tau-1)/(e^{\tau_{\max}}-1), \quad j=0, \dots, n_\tau-1. \quad (3.1)$$

The values are generated independently for each triplet (d_2, d_3, τ) , τ starting from 0 (then $t_{\max}=0$) and increasing to its maximum value, taking the previous $t_{\max}$ as a starting point. During program execution the starting value is found by determining the three nearest (d_2, d_3) points in the table and making a linear interpolation on the three values at these points, cf. fig 3. This is done for the nearest table τ -values below and above and finally a linear interpolation is done between those values. During a number of test runs it took on average 9 function evaluations to get from this value to the true $t_{\max}$ with a relative error less than 10^{-4} .

The programs were implemented on a Atlas-10 (Fujitsu M380), a 32 bit, 15 MIPS machine, and run on a 16^4 lattice gauge field configuration, sliced in one of the dimensions (time). At any moment there are 4 time-slices in the machine and the total program required 6 Mbyte of memory. The slices are transported between memory and disk by asynchronous IO. To go once through the whole lattice requires on average 222 seconds, which is 847 μ s/link.

4. Discussion

To cool one configuration to a point where the asymptotic action can be determined requires 200 to 400 sweeps through the lattice, as illustrated in fig. 4. The results are expressed in terms of the mean plaquette, the action (1.4) divided by the number of plaquettes, which for a 16^4 lattice is 393216. The asymptotic limit is found in the following way. Fit the differences of the mean plaquette p_n over the last 30 sweeps to the formula

$$d_n = - \left(\frac{n_0}{n} \right)^a \quad (4.1)$$

where n is the sweep-number. The predictions for the asymptotic mean plaquette,

$$p_{\infty} = p_n - \frac{n}{a-1} \left(\frac{n_o}{n} \right)^a, \quad (4.2)$$

turn out to increase as the maximum n to which is fitted increases. This is illustrated in table 1. Thus the last p_{∞} -prediction may be taken as a lower bound for p_{∞} . Also p_{∞} is bounded from above by the last p_n . The limit found in this fashion for the configuration depicted in fig. 4 is

$$.0001331 < p_{\infty} < .0001336. \quad (4.3)$$

The mean plaquette resulting from one $SU(3)$ - instanton is

$$.000033466, \quad (4.4)$$

so 4 instantons would give a value which is very compatible with the value found.

To actually deduce the η' -mass, this procedure has to be repeated on at least 20 configurations. This work is in progress and results will be reported elsewhere.

References

- [1] S. Coleman, in *The Whys of Subnuclear Physics*, (Erice 1977), ed. A. Zichichi (Plenum Press, New York, 1979).
- [2] M.E. Peskin, in *Recent Advances in Field Theory and Statistical Mechanics* (Les Houches 1982), eds. J.-B. Zuber and R. Stora (Elsevier Science Publ. B.V., Amsterdam, 1984).
- [3] G.A. Christos, *Chiral Symmetry and the U(1) Problem*, Australian National University at Canberra, preprint (1984).
- [4] G.'t Hooft, *Phys. Rev. Lett.* 37 (1976) 8; *Phys. Rev. D* 14 (1976) 3432; *Phys. Rev. D* 18 (1978) 2199.
- [5] E. Witten, *Nucl. Phys. B* 156 (1979) 269.
- [6] G. Veneziano, *Nucl. Phys. B* 159 (1979) 213.
- [7] P. Woit, *Phys. Rev. Lett.* 51 (1983) 638.
- [8] B. Berg and M. Luscher, *Nucl. Phys. B* 190 [FS3] (1981) 412.
- [9] B. Berg, *Phys. Lett.* 104B (1981) 475.
- [10] D. Petcher and M. Luscher, *Nucl. Phys. B* 225 [FS9] (1983) 53.
- [11] Y. Iwasaki and T. Yoshie, *Phys. Lett.* 125B (1983) 197; *Phys. Lett.* 131B (1983) 159.
- [12] J. Polonyi, *Topological Charge of the Lattice CP^{N-1} Model*, preprint ILL-(TH)-83-3; *Phys. Rev. D* 29 (1984) 716.
- [13] I.A. Fox, J.P. Gilchrist, M.L. Laursen and G. Schierholz, *Phys. Rev. Lett.* 54 (1985) 749.
- [14] A.A. Belavin, A.M. Polyakov, A.S. Schwarz, Yu.S. Tyupkin, *Phys. Lett.* 59B (1975) 85.
- [15] J.-M. Drouffe and J.-B. Zuber, *Phys. Rep.* 102 (1983) 1.
- [16] K. Wilson, in *New Phenomena in Subnuclear Physics* (Erice 1975) ed. A. Zichichi, (Plenum Press, New York, 1977); *Phys. Rev. D* 10 (1974) 2445.
- [17] M.J.D. Powell, *Comp. Journ.* 7 (1965) 303.
- [18] A. Patel, *Monte-Carlo Renormalization Group for Lattice QCD*, (Caltech, 1984), thesis, unpublished.

Table 1

last sweep	a	n_o	$p_{\infty} \times 10^4$
300	6.73	425	1.3203
310	7.29	413	1.3264
320	7.43	410	1.3274
330	7.50	409	1.3281
340	7.71	406	1.3291
350	7.72	406	1.3293
360	7.86	405	1.3297
370	8.05	403	1.3302
380	8.26	402	1.3306
390	8.17	403	1.3305
400	8.28	402	1.3307

Results of a fit to formula (4.1)

Figure Captions

1. Distribution of $|\tau|$ for a random configuration.
2. Distribution of d_2 and d_3 for a random configuration.
3. Division of (d_2, d_3) plane indicating the points used for the look-up table (intersections) and the two types of triangles used for interpolation (shaded).
4. Mean plaquette p_n versus the number of cooling sweeps.

fig. 1

fig. 2

Fig. 3

FIG. 4