Overrelaxed operators in lattice gauge theories

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For operators in lattice gauge theories linear in the link variables we propose improved estimators, obtained from a microcanonical integration of statistically independent links. We give explicit analytic expressions for the SU(2) and the SU(3) cases and we compare the method with the canonical integration based on the multihit technique.

The statistical accuracy of the estimates in a Monte Carlo simulation of lattice gauge theories can be improved by a wise choice of the estimators employed. Indeed, as has been observed already a long time ago, there is in general a set of "equivalent" operators all having the same average, but different mean square deviations. Those where the lattice is the smallest possible constitute the best estimators for a calculation with limited statistics. To fix our notations, we consider a gauge theory defined on a lattice in terms of link variables taking values in an SU(N) group. The action S will be of the Wilson-type, i.e. a sum over all plaquettes defined as the real part of the trace of the ordered product of four links around an elementary square.

For operators which are linear in the gauge links, it was proposed [1,2] to replace the value of a link with its average calculated for fixed values of the neighbouring links. In equations:

$$\langle L(\ldots U_{ab} \ldots)\rangle = \langle L(\ldots \langle U\rangle_{ab} \ldots)\rangle, \qquad (1)$$

with

$$\langle U\rangle_{ab} = \frac{\int dU\, U_{ab}\, \exp\{-\beta S(\mathrm{Re}\,\mathrm{Tr}[\,UM\,])\}}{\int dU\, \exp\{-\beta S(\mathrm{Re}\,\mathrm{Tr}[\,UM\,])\}}, \qquad (2)$$

with M the sum of the incomplete plaquettes (staples) which have the given link in common. Of course such a substitution is legitimate only for those links which

are statistically independent, i.e. which do not appear in the same plaquette.

The idea was applied first [2] to the calculation of correlations of Polyakov loops in SU(3) and the results were so successful to allow to determine for the first time the correct value of the string tension at $\beta = 6$ on a $10^3 \times 20$ lattice. This would have been impossible with ordinary Polyakov loops because of the great statistical noise affecting the correlations at distances larger than three or four lattice spacings.

An explicit form for the exact average of the link in SU(3) is not available and one has to use the "multihit" technique. It consists of performing many Monte Carlo steps on the same link, of storing the values obtained and of estimating from their average the true average value. Typically 10 to 15 hits per point are used with satisfactory results. The same calculation was repeated for the SU(2) group where again the multihit improvement proved to be very effective, although in this case an exact expression can be written in terms of a ratio of Bessel functions.

In this letter we propose to replace the link with its partial average over those orbits in the group space which leave the sum of plaquettes containing that link – i.e. the energy – invariant. We perform a micro-canonical integration hoping that – at equilibrium – it represents a relevant sampling of the canonical one. The calculation of the microcanonical average in

SU(2) is straightforward:

$$\langle U \rangle = \frac{M^\dagger}{\text{Tr}[M^\dagger M]} \text{Tr}[UM], \tag{3}$$

where we have used the same notation of eq. (2).

As a test, we have used the expression above in the calculation of the correlation of Polyakov loops at $\beta = 2.4$ on a 8^4 lattice. The results obtained from an average over 50 configurations each separated by 50 decorrelating configurations (we have used a standard heat bath) are reported in fig. 1: for comparison the results without the improvement are also shown. The microcanonical integration compares well with the full integration which was presented in ref. [3].

The real issue is a quantitative comparison with the multihit technique. In order to do this we have defined a distance of a complex SU(2) matrix A from another matrix B as

$$d(A, B) = \frac{1}{2} \left(\sum_{i=0}^{3} (a_i - b_i)^2 \right)^{1/2}, \tag{4}$$

with

$$A = a_0 I + i a_i \sigma_i, \quad B = b_0 I + i b_i \sigma_i, \tag{5}$$

where we have adopted a standard parametrization for the matrices (I is the unity matrix and σ_i are the Pauli matrices). Fig. 2 reports the histogram of 50 different cases of the distance from the full average of the link itself (dashed), of the link averaged over

10 (heat bath) hits (dotted) and of the microcanonical average (full). The latter appear to be the closest to the full average. It corresponds to about 25 hits of the multihit procedure. The links considered in this calculation come from a configuration thermalized at $\beta = 2.4$.

An analytic expression for a microcanonical average can be obtained not only in SU(2), but in general for SU(N) groups. We give a detailed description for the SU(3) case. We want to calculate the quantity

$$\langle U_{ab} \rangle =$$

$$\frac{\int dU\, U_{ab}\, \exp\{-\beta S(\text{Re Tr}[UM])\}}{\int dU\, \exp\{-\beta S(\text{Re Tr}[UM])\}} \bigg|_{\text{Re Tr}[UM]=\text{const.}} . \tag{6}$$

The matrix M can be decomposed as

$$M = M \frac{1}{(M^\dagger M)^{1/2}} (M^\dagger M)^{1/2} \equiv O(M^\dagger M)^{1/2} \equiv OH, \tag{7}$$

where O is a U(3) matrix with a complex determinant of modulus 1 and H is a hermitean matrix. The matrix O can be reduced to an SU(3) matrix by multiplying it with a matrix $I(\alpha)$ proportional to the unity matrix with $\det[I(\alpha)] = \det[O^\dagger]$. Therefore

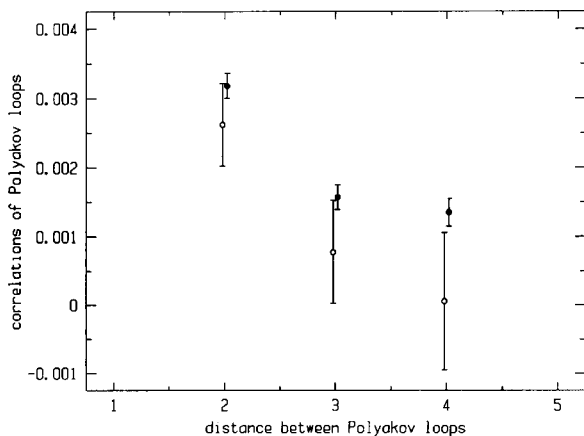$$M = \tilde{O} I(\alpha)^\dagger H, \tag{8}$$

Fig. 1. The correlations of Polyakov loops as function of the distance for the standard operators (○) and for the improved operators (●), for the SU(2) gauge theory at $\beta = 2.4$.
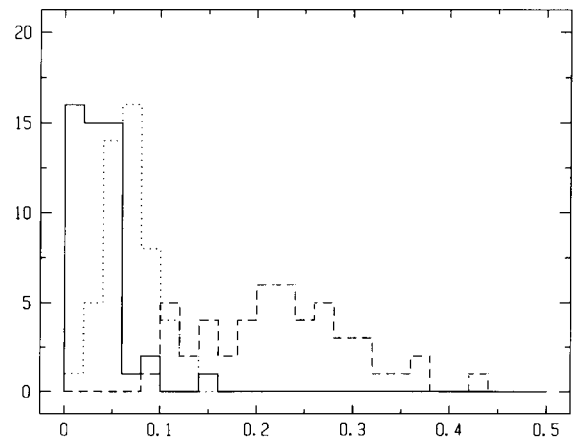

Fig. 2. The distance from the average, defined in the text, of the original link (dashed), the average performed over 10 heat bath Monte Carlo hits (dotted), the microcanonical average (full), for the SU(2) gauge theory at $\beta = 2.4$.

where $\tilde{O} = OI(\alpha)$ is now an SU(3) matrix. The matrix H can be diagonalized by a unitary transformation,

$$H = V^\dagger DV. \tag{9}$$

We obtain the following identity:

$$\mathrm{Tr}[\,UM\,] = \mathrm{Tr}[\,VU\tilde{O}V^\dagger I(\alpha)^\dagger D\,]. \tag{10}$$

The invariance of the group measure under a unitary transformation leads to

$$\langle U \rangle = \frac{\int dU'\, V^\dagger U'V\tilde{O}^\dagger \exp(-\beta S\{\mathrm{Re}\,\mathrm{Tr}[\,U'I(\alpha)^\dagger D]\})}{\exp(-\beta S\{\mathrm{Re}\,\mathrm{Tr}[\,U'I(\alpha)^\dagger D]\})}$$

$$= V^\dagger \frac{\int dU'\, U' \exp(-\beta S\{\mathrm{Re}\,\mathrm{Tr}[\,U'I(\alpha)^\dagger D]\})}{\int dU' \exp(-\beta S\{\mathrm{Re}\,\mathrm{Tr}[\,U'I(\alpha)^\dagger D]\})}\, V\tilde{O}^\dagger. \tag{11}$$

The trace in the exponent depends upon the diagonal elements of U' only. The non-diagonal elements of U' average to zero in the microcanonical integration. This can be proven by considering that the measure and the exponential are invariant under three "reflections" of non-diagonal elements. Denoting by U_{ab} the matrix elements, the reflections are

(1) $U^r_{12} = -U_{12}, \quad U^r_{21} = -U_{21},$

$\quad\quad U^r_{13} = -U_{13}, \quad U^r_{31} = -U_{31};$ (12)

(2) $U^r_{12} = -U_{12}, \quad U^r_{21} = -U_{21},$

$\quad\quad U^r_{23} = -U_{23}, \quad U^r_{32} = -U_{32};$ (13)

(3) $U^r_{13} = -U_{13}, \quad U^r_{31} = -U_{31},$

$\quad\quad U^r_{23} = -U_{23}, \quad U^r_{32} = -U_{32}.$ (14)

Any two of the above reflection properties imply that the non-diagonal elements of U' average to zero. Similar arguments can be extended to a generic SU(N) group.

The microcanonical average in SU(3) reads

$$\langle U \rangle_{mc} = V^\dagger [\,VUOV^\dagger]_{diag} VO^\dagger, \tag{15}$$

where the subscript diag means that the off-diagonal elements of the matrix in brackets are set to zero. In eq. (15) we have used the matrix O instead of $\tilde{O}$ because $I(\alpha)$ is proportional to the unity matrix, commutes with any matrix and with the averaging operation and disappears from the final expression. When specialized to the SU(2) case, the expression in eq. (15) can be seen to represent only a partial microcanonical integration.
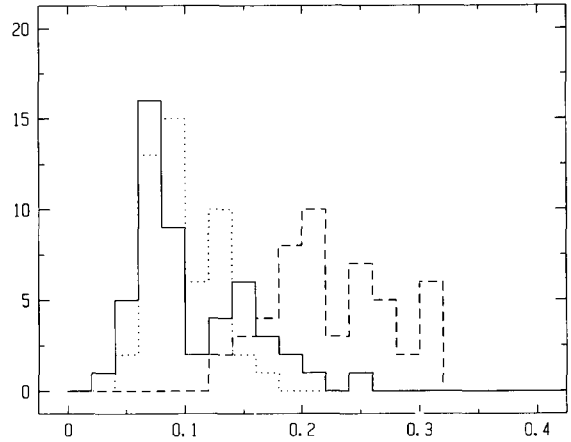

Fig. 3. The same as in fig. 2 for the SU(3) group at $\beta = 5.6$.

Defining the distance between two matrices A and B in SU(3) as

$$d(A, B) = \left(\frac{1}{18} \sum_{i,j} |A_{ij} - B_{ij}|^2\right)^{1/2}, \tag{16}$$

we can extend to SU(3) the comparison with the multihit technique done for SU(2). We take links from a configuration thermalized at $\beta = 5.6$. The results are presented in fig. 3. The SU(3) partial microcanonical average turns out to be more effective than 10 hits performed with the Cabibbo and Marinari (CM) algorithm [4] while the computer time requirement is equivalent to roughly one hit only.

The construction presented in this paper provides also an exact expression for a "reflected" link which has the same energy as the original one:

$$U_R = V^\dagger [\,VUOV^\dagger]_r VO^\dagger \tag{17}$$

where the subscript r means that to the matrix in brackets one of the operations in eqs. (12), (13), (14) has been applied. The reflected link could be used for the construction of an exact overrelaxed Monte Carlo algorithm [5].

References

[1] G. Parisi, Phys. Rep. 103 (1984) 203.
[2] G. Parisi, R. Petronzio and F. Rapuano, Phys. Lett. B 128 (1983) 418.
[3] A. Billoire and E. Marinari, Phys. Lett. B 139 (1984) 399.
[4] N. Cabibbo and E. Marinari, Phys. Lett. B 119 (1982) 387.
[5] M. Creutz, Phys. Rev. D 36 (1987) 515.