GROUP THEORY AND LATTICE GAUGE FIELDS

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ABSTRACT

Lattice gauge theory, formulated in terms of invariant integrals over group elements on lattice bonds, benefits from many group theoretical notions. Gauge invariance provides an enormous symmetry and powerful constraints on expectation values. Strong coupling expansions require invariant integrals over polynomials in group elements, all of which can be evaluated by symmetry considerations. Numerical simulations involve random walks over the group. These walks automatically generate the invariant group measure, avoiding explicit parameterization. A recently proposed overrelaxation algorithm is particularly efficient at exploring the group manifold. These and other applications of group theory to lattice gauge fields are reviewed in this talk.

At first, lattice gauge theory seems like a natural topic for discussion at a conference on group theory. Indeed, in our large scale numerical simulations we store and manipulate thousands of group elements in computer memory. On the other hand, much of this work is rather tedious writing and debugging of computer programs. When actually working on these topics the abstract nature of much of group theory seems rather remote. On still further reflection, however, we actually use many consequences of the fact that our variables are group elements. It is some of these that I will try to emphasize in this talk.

I begin by defining lattice gauge theory [1]. For simplicity I start with a four dimensional hypercubic lattice. For definiteness, assume that the lattice has N^4 sites and has periodic boundary conditions. For every ordered nearest neighbor pair of sites (i, j) on this lattice, I have a bond variable U_{ij} which is an element of the gauge group G. To study the theory of the strong interactions, where the gauge fields are the gluons which bind quarks into hadrons, we are interested in the gauge group $SU(3)$. For the bond considered in the reverse direction, the associated element is $U_{ji} = U_{ij}^{-1}$. I will assume that G is a compact unitary group. Thus I consider a configuration space which consists of $4 \times N^4$ group elements.

Associated with every configuration of this system is an action

$$S = \sum_p \left(1 - \frac{1}{n} \text{Re } \text{Tr} \, U_p\right). \tag{1}$$

Here the trace is in some representation, usually the fundamental, of the gauge group, and n is the dimension of the matrices in that representation. The sum is over all elementary squares, or "plaquettes," p, and U_p denotes an ordered product of the fundamental link variables around the given plaquette. Because of the trace it does not matter on which corner of the plaquette the product starts. Because of the real part being taken in Eq. (1) and because the group is unitary, the direction taken around the square is unimportant.

The next step is to place the action into a Boltzmann weight and study the corresponding statistical mechanics of this system of group elements. Thus I consider

the partition function

$$Z = \int (dU) \ e^{-\beta S}. \tag{2}$$

The parameter β is proportional to the inverse square of the bare gauge coupling g_0 used in conventional perturbative studies. For the gauge group $SU(n)$ the relation is

$$\beta = 2n/g_0^2. \tag{3}$$

The expectation value for some function F of the gauge variables is

$$\langle F \rangle = Z^{-1} \int (dU) \ F(U) \ e^{-\beta S}. \tag{4}$$

In these equations the integration is to be taken over all the link variables using the invariant group measure. For compact groups this measure satisfies

$$\int dg f(g) = \int dg f(gg') = \int dg f(g'g) = \int dg f(g^{-1}) \tag{5}$$

where $f(g)$ is an arbitrary function over the group. The measure is normalized such that

$$\int dg \ 1 = 1. \tag{6}$$

Eq. (5) can be schematically written $dg = d(gg') = d(g'g) = d(g^{-1})$.

In addition to the gauge fields on the links, one can readily add matter fields which conventionally reside on the lattice sites. The interaction with the gauge fields is easily constructed to display the gauge symmetries to be discussed below. For simplicity, however, I will ignore such fields in this talk.

This completes the formal definition of a lattice gauge theory. The motivations for looking at this system can be found in the many reviews of the topic, for example ref. [2]. Briefly, the classical continuum limit of the above action reproduces the Yang Mills fields and the integration over the links gives a regularized Feynman path integral for the quantization of the system.

For the quantum theory the issue is less clear. I will take the point of view that the continuum limit of lattice gauge theory, if it exists, is a definition of quantized gauge fields. The phenomenon of asymptotic freedom does give some

useful information on how to take this limit. As the lattice spacing a is reduced we will encounter the well known divergences of quantum field theory and the coupling must be renormalized. This variation of the bare coupling with cutoff is given by the renormalization group function

$$a\frac{\partial g_0}{\partial a} = \gamma\left(g_0\right) = \gamma_0 g_0^3 + \gamma_1 g_0^5 + \cdots \tag{7}$$

Integrating this and expressing the lattice spacing as a function of the bare coupling gives

$$a = \frac{1}{\Lambda}\left(g_0^2\gamma_0\right)^{-\gamma_1/2\gamma_0^2} e^{-1/2\gamma_0 g_0^2} \times \left(1 + \mathcal{O}\left(g_0^2\right)\right) \tag{8}$$

where Λ is an integration constant and sets the overall scale of the theory.

When working on the lattice it is quite natural to measure masses in units of the lattice spacing. If a particle has a finite mass m in the continuum limit, then the dimensionless combination ma will show an exponential decrease with the inverse coupling as in Eq. (8). The coefficient of this "scaling" behavior gives the particle mass in units of Λ. Note that the factor of Λ will drop out of any mass ratios. Indeed, in the continuum limit the pure gauge theory should make parameter-free predictions for all dimensionless observables. When quarks are added to the theory the only parameters are the quark masses (in units of Λ).

The action in Eq. (1) has an enormous symmetry. Suppose we associate an arbitrary group element g_i with every site i on our lattice. Using these, we can construct a new link element on each bond

$$U'_{ij} = g_i U_{ij} g_j^{-1}. \tag{9}$$

Since the action involves the trace of link variables multiplied around closed loops, the factors of g will cancel in the calculation of the action for the new links, which will therefore give exactly the same action as the old. This exact local symmetry is the gauge symmetry of the model. On our N^4 site lattce, the symmetry group is the gauge group raised to the N^4 power.

For good observables we should look for gauge invariant operators. One such is the trace of the product of link variables around a closed loop. The expectation of

this is the famous Wilson loop. Confinement in the pure gauge theory is signaled by an exponential decrease with the minimal area enclosed by the loop. The coefficient of this area law is a non-local order parameter which is useful for distinguishing certain phases of lattice gauge models.

The area law for Wilson loops arises naturally in the strong coupling expansion. In that approach group theory plays a major role. When the bare coupling becomes large, the parameter β is small and one can consider a power series expansion of the Boltzmann weight $e^{-\beta S}$. Any term in this expansion will involve various powers of the link variables, which must be integrated over. For $SU(n)$ the resulting integrals can be done using a set of graphical rules which I will not go into here [3]. The net result for the expectation of a Wilson loop is that terms in the strong coupling expansion will all vanish until enough powers of β are taken so that a minimal surface with the loop as boundary can be tiled with plaquettes taken from the Boltzmann factor. This factor of β raised to the area of the loop is precisely the exponential suppression signaling confinement.

For the past several years research in lattice gauge theory has been dominated by Monte Carlo simulations. The basic idea is to approximate the integral in Eq. (4) by a sum over a finite number of configurations of the system with a weighting proportional to the Boltzmann factor $e^{-\beta S}$. Using the formal analogy with statistical mechanics, we wish to find a set of configurations typical of thermal equilibrium.

For simplicity in the following discussion, consider just a single group element U. Assume we wish to stochastically pick elements with a probability distribution

$$P_{eq}(U) \propto e^{-\beta S(U)} \tag{10}$$

where $S(U)$ is some prescribed action. The differential measure to be used here is the same invariant measure used for integration above.

For groups such as $SU(2)$ where the explicit measure is rather simple, it is not difficult to generate elements with a particular distribution. At first it would seem that for other groups with more complicated invariant measures it might be

quite difficult to generate elements with an arbitrary distribution. It turns out, however, that by doing a random walk over the group manifold this can be quite easy.

Given an ensemble of group elements uniformly distributed over the group, the invariance of the measure insures that if all elements in this set are multiplied by some fixed group element, then the new ensemble will also be uniform. This fact provides a way to obtain such a uniform distribution. Suppose we have a set of factors which upon repeated multiplication can cover the group. In a practical simulation these factors could be stored in a finite table. Then we can construct a Markov chain of group elements by starting with an arbitrary element and repeatedly multiplying the current element U by randomly chosen factors. Asymptotically this sequence will uniformly cover the group.

Actually, rather than a uniform covering, Eq. (10) asks for a weighted distribution. This can be readily accomplished by modifying the above Markov chain. This is usually done by an accept/reject procedure as suggested by Metropolis *et al.* [4]. To proceed it is useful to introduce an auxiliary group element V. With this element I associate some simple action $\bar{S}(V)$. Suppose further that this action satisfies $\bar{S}(V) = \bar{S}(V^{-1})$. A particularly simple choice in practice is

$$\bar{S}(V) = -k\operatorname{Re}\operatorname{Tr}(V) \tag{11}$$

I now define a "Hamiltonian"

$$H(U,V) = S(U) + \bar{S}(V) \tag{12}$$

In terms of this, I wish to find pairs of group elements U and V with probability

$$P_{eq}(U,V) \propto e^{-\beta H} \tag{13}$$

Ignoring the auxiliary variable V, I have an appropriate distribution for U. I am pursuing an analogy where U corresponds to some canonical variable x and V to a conjugate momentum p. The action $S(U)$ corresponds to a potential energy $V(x)$ and the Hamiltonian to $V(x) + p^2/2$.

Now consider a simultaneous trial change of both U and V to

$$U' = V F (U) U$$
$$V' = \left(F (U') V F (U) \right)^{\dagger}. \tag{14}$$

Here $F (U)$ is a group element which can have an arbitrary dependence on U. I refer to it as a "driving force." This trial change is then to be accepted with a conditional probability

$$P \left(U, V \to U', V' \right) = \min \left[1, e^{-\beta \left(H' - H \right)} \right]. \tag{15}$$

If the change is rejected, then U and V retain their old values. This scheme of conditionally accepting trial changes guarantees that an equilibrium ensemble remains in equilibrium. Indeed, it can be readily verified that this is sufficient to insure that a non-equilibrium ensemble will be brought closer to equilibrium.

The change of variables indicated in Eq. (14) has several useful properties. First, it is easily inverted by merely iterating the equation. Second, the transformation preserves volumes in the direct product space of the group with itself. That is, given an arbitrary function $h (U, V)$, we can repeatedly use group invariance to derive

$$\int dU \; dV \; h (U, \; V) =$$
$$\int dU \; dv \; h \left(U, \; V^{\dagger} \right) =$$
$$\int dU \; dV \cdot h \left(U, \; (F (U) V)^{\dagger} \right) =$$
$$\int dU \; dV \; h \left(V U, \; (F (V U) V)^{\dagger} \right) = \tag{16}$$
$$\int dU \; dV \; h \left(V F (U) U, \; (F (V F (U) U) \; V \; F (U))^{\dagger} \right) =$$
$$\int dU \; dV \; h \left(U', V' \right)$$

or, schematically, $dU \; dV = dU'dV'$. Note that no explicit representation of the group measure is needed.

This preservation of phase space volumes gives rise to a useful identity on the corresponding energy change. Consider the partition function

$$Z = \int dU' \; dV' \; e^{-\beta H (U', V')}. \tag{17}$$

Changing variables to U and V and adding and subtracting $H(U,V)$ in the exponent gives

$$Z = \int dU \, dV \, e^{-\beta H} \, e^{-\beta(H'-H)} \qquad (18)$$

where H and H' denote $H(U,V)$ and $H(U',V')$, respectively. Dividing by Z, we find

$$\langle e^{-\beta(H'-H)} \rangle = 1 \qquad (19)$$

where the expectation is over all U and V with the equilibrium distribution of Eq. (13). Because the exponential function is convex, Eq. (19) immediately implies

$$\langle H' - H \rangle \geq 0 \qquad (20)$$

with equality only possible if the dynamics is exactly energy conserving. If we consider small changes in energy, a useful consequence of Eq. (18) follows by expanding the exponential

$$\langle H' - H \rangle = \frac{\beta}{2} \langle (H'-H)^2 \rangle + \mathcal{O}\left((H'-H)^3 \right). \qquad (21)$$

After performing the above Monte Carlo process on the U and V variables, it is generally advantageous to "refresh" the auxiliary variables V. This can be done by another Monte Carlo process on the V variables alone, or, in the case when there are several V elements, randomly permuting them.

This framework describes a large class of algorithms. If the force $F(U)$ is always taken to be the identity element, the procedure is the standard unbiased Metropolis *et al.* [4] algorithm with

$$\begin{aligned} U' &= VU \\ V' &= V^\dagger. \end{aligned} \qquad (22)$$

In this case the V variables are usually selected randomly from a table which should contain the inverse of each of its elements.

Another potentially useful scheme for picking the driving force was discussed in refs. [5–6]. This approach is a generalization of the overrelaxation ideas discussed in ref. [7]. Suppose there is some straightforward way to find a group element

U_0 which approximately minimizes the action $S(U_0)$. Suppose further that U_0 is obtained with no explicit dependence on the current element U. If we select

$$F(U) = \left(U_0 U^{-1}\right)^2,\tag{23}$$

then the trial change is

$$U' = V U_0 U^{-1} U_0$$
$$V' = \left(F^{-1} V F\right)^{\dagger}.\tag{24}$$

In some sense the new U lies centered about the "opposite side" of U_0 from U. The noise introduced by V plays a rather minor role and can be eliminated by taking $V = I$.

This choice of trial update produces a rather large change in U while, assuming the action is reasonably symmetric around U_0, resulting in only a rather small change in the action. Thus one simultaneously obtains a high acceptance rate and a rapid flow through configuration space. In addition, recent analyses by Adler [8] and Neuberger [9] indicate that overrelaxation can help reduce the increase of correlation times as a critical point is approached. Tests with this algorithm [6], [10] indicate a possible savings of order a factor of three in computer time over the conventional Metropolis *et al.* [4] algorithm for pure $SU(3)$ gauge theory.

An interesting class of algorithms arises if we take $\bar{S}(V)$ so that the distribution of V is highly peaked near the identity. It is then possible to choose F so that changes in the energy are of order the cube of the change in the group element. To see this more explicitly, parameterize the link variables

$$U = e^{iA \cdot \lambda}\tag{25}$$

where the matrices λ generate the Lie algebra for the group. Now take for the driving force

$$F = exp\left(-i\epsilon\lambda \cdot \frac{\partial S}{\partial A}\right),\tag{26}$$

and for the auxiliary action take

$$\bar{S}(V) = \frac{1}{2\epsilon}\mathrm{Re}\,\mathrm{Tr}\,V.\tag{27}$$

This choice will make

$$H' - H = \mathcal{O}\left(\epsilon^{3/2}\right) \tag{28}$$

which implies, by Eq. (21),

$$\langle H' - H \rangle = \mathcal{O}\left(\epsilon^3\right) \tag{29}$$

Thus for small ϵ we expect a rather high acceptance rate. Leaving off the accept/reject step gives an approximate algorithm which becomes more exact as the peaking of V around the identity becomes stronger. With frequent refreshing of the V distribution, we obtain a discretization of the Langevin equation. In this discretization, ϵ plays the role of the time step and V provides the noise term. The simple uncorrected Langevin approach to lattice gauge theory has been advocated in refs. [11–12]. Making the algorithm exact with an accept-reject step was proposed in reference [13]. This implementation of the Langevin evolution using group elements for the noise was recently tested for $SU(3)$ lattice gauge theory [14].

An interesting variation is the hybrid approach originally discussed in [15]. The addition of the accept reject step to make this algorithm exact was discussed in reference [16]. Here we consider Eq. (14) followed by an inversion of V. This combination is then iterated N_{mic} times before applying the accept-reject procedure. This iteration generates an approximately microcanonical trajectory which still exactly preserves areas in phase space. For the driving force use Eq. (26) and let N_{mic} be of order $1/\sqrt{\epsilon}$. After each trajectory and accept-reject step, the V matrices should be refreshed. The advantage of this procedure is that on a trajectory the random walk of the Langevin approach is replaced by a continued motion in the direction of the slowly evolving V matrices. This gives a more rapid final flow through phase space. This is partially compensated by the need for a smaller ϵ, because now a given trajectory has

$$H' - H = \mathcal{O}\left(\epsilon\right)$$
$$\langle H' - H \rangle = \mathcal{O}\left(\epsilon^2\right) \tag{30}$$

Nevertheless there is a net overall gain.

I will now make a few brief remarks on including fermionic fields in our simulations. In this case the generic partition function becomes

$$Z = \int (dU) (d\psi^* d\psi) \, exp \left(-S_0 (U) - \psi^* M \psi\right) \tag{31}$$

where S_0 is the pure gauge actgion, ψ^* and ψ are anticommuting variables and M is some matrix coupling the fermions and gauge fields. To set up a Monte Carlo simulation, the fermionic fields are integrated out and replaced by an integral over commuting fields interacting with the inverse of the fermionic matrix. More precisely, Eq. (31) is rewritten

$$\begin{aligned} Z &= \int (dU) \det (M) \, e^{-S_0} \\ &= \int (dU) (d\phi) \exp \left(-S_0 - \left(M^{-1}\phi\right)^2 /2\right). \end{aligned} \tag{32}$$

The difficulty with this is that $M^{-1}\phi$ is rather tedious to calculate. All practical schemes perform this inversion only once per sweep of the gauge variables. While most schemes make a small step approximation, this can be avoided by a global accept-reject step following an approximate full sweep. This will still require a small step size to maintain a reasonable acceptance, but eliminates systematic errors. The value of the Langevin and hybrid approaches become particularly clear in these schemes. A recent analysis [17] shows that an unbiased global updating requires computer time growing as the square of the system volume. The Langevin approach reduces this to a $V^{4/3}$ growth, and the corrected hybrid scheme gives a $V^{5/4}$ behavior. Recently there has been extensive activity testing these algorithms.

To conclude, I hope I have been able to show you that lattice gauge theory is not just writing computer programs, but involves some elegant group theory as well. The group theory we use, however, differs somwhat from that seen in particle theory. In particular, details of higher representations of the gauge group only play a minor role, while the properties of invariant group integration are crucial.

REFERENCES

1. K. Wilson, Phys. Rev. D10, 2445 (1974).

2. M. Creutz, *Quarks, Gluons and Lattices* (Cambridge Univ. Press 1983).

3. M. Creutz, J. Math. Phys. $\underline{19}$, 2043 (1978).

4. N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. $\underline{21}$, 1087 (1953).

5. F. R. Brown and T. J. Woch, Phys. Rev. Lett. $\underline{58}$, 2394 (1987).

6. M. Creutz, Phys. Rev. $\underline{D36}$, 515 (1987).

7. S. L. Adler, Phys. Rev. $\underline{D23}$, 2901 (1981); C. Whitmer, Phys. Rev. $\underline{D29}$, 306 (1984); Princeton University PhD thesis (1984).

8. S. L. Adler, Phys. Rev. $\underline{D37}$, 458 (1988).

9. H. Neuberger, Phys. Rev. Letters, $\underline{59}$, 1877 (1987).

10. R. Gupta, G. Kilcup, A. Patel, S. Sharpe, and P. de Forcrand, preprint LA-UR-88-824 (1988).

11. G.G. Batrouni, G.R. Katz, A.S. Kronfeld, G.P. Lepage, B. Svetitsky and K.G. Wilson, Phys. Rev. $\underline{D32}$, 2736 (1985).

12. A. Ukawa and M. Fukugita, Phys. Rev. Lett. $\underline{55}$, 1854 (1985).

13. R. Scalettar, D. Scalapino, and R. Sugar, Phys. Rev. $\underline{B34}$, 7911 (1986).

14. M. Creutz, H. Gausterer, and S. Sanielevici, BNL preprint (1988).

15. S. Duane and J. Kogut, Phys. Rev. Lett. $\underline{55}$, 2774 (1985); Nucl. Phys. $\underline{B275}$, 398 (1986).

16. S. Duane, A. K. Kennedy, B.J. Pendleton and D. Roweth, Phys. Lett., $\underline{195}$, 2 (1987).

17. M. Creutz, Phys. Rev. $\underline{D38}$, 1228 (1988).