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# NUMERICS FOR NOVICES:

## Computational methods for lattice gauge theory

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**Abstract**

A brief review and summary is given of recent progress in the application of microcanonical ensemble techniques to lattice gauge theory.

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## 1. Prolegomena

The numerical analysis of lattice gauge theories[1] has provided a new viewpoint for the examination of the nonperturbative structure of quantum field theory. There is now reason to hope that hadronic physics will soon be understood at a quantitative level[2,3]; additionally non-perturbative studies[4] of the weak interaction may lead to phenomenologically useful results such as a bounded or calculable Higgs mass. Before any of these goals can be realized, however, the numerical methods currently in use must be perfected. It is therefore now appropriate to review recent progress in this direction.

One approach which seems to be of general use is the so-called "microcanonical ensemble" method for lattice gauge theory. This idea was originally developed and applied to U(1), SU(2), and SU(3) lattice gauge theories by Aneesur Rahman and the present author,[5,6] and has since been applied by others to a wide variety of problems.[7-12] Due to space limitations, this review will focus only on recent progress in developing this method; other methods are discussed elsewhere[2,3].

In the microcanonical-ensemble formulation of lattice gauge theory, expectation values are calculated by solving a large set of coupled ordinary (as opposed to partial) differential equations. One feature of this method is that it is deterministic, that is, no random numbers are needed to generate configurations. The microcanonical-ensemble formulation (or one of its derivatives[10]) may also be most appropriate when calculations are performed by

parellel-processing techniques (such as on an array processor), for differential equations can be integrated simultaneously. Typically in a Monte Carlo calculation the lattice cannot be updated in a single pass because each link interacts with its neighbors, and so a simultaneous update of link and neighbor would violate detailed balance.

## 2. Review of the microcanonical ensemble

Recall how expectation values are calculated in the usual[1] approach to quantum field theory on a lattice. The central assumption of this formalism is that expectation values of functionals O of a finite number of fields $\{\phi\}$ on a Euclidean lattice can be extrapolated to a continuum limit. If the action is denoted by $S\{\phi\}$, such expectation values are defined by

$$\langle O \rangle_{\text{lattice}} \equiv Z^{-1}_{\text{lattice}} \int D\,\phi \;\; O\{\phi\}\; e^{-S\{\phi\}} \tag{1a}$$

where

$$Z_{\text{lattice}} \equiv \int D\,\phi \;\; e^{-S\{\phi\}} \tag{1b}$$

and

$$\int D\,\phi \equiv \prod_{n=1}^{N} \int d\,\phi_n \quad . \tag{1c}$$

These standard formulae, Eqs. (1), can be cast in a form which is obviously equivalent to a classical canonical ensemble. Recall that any quantity which is independent of all the $\{\phi\}$ can be added to the action $S\{\phi\} \equiv \beta\, V\{\phi\}$ without changing the expectation value of any functional of the $\{\phi\}$ alone. We chose[5,6] to add a



quantity $\beta T\{p\}$, where $T\{p\}$ is defined by

$$T\{p\} \equiv \frac{1}{2} \sum_{n=1}^{N} p_n^{\,2} \tag{2}$$

so that

$$\langle O \rangle_{\text{lattice}} = \langle O \rangle_{\text{canonical}} \tag{3a}$$

where

$$\langle O \rangle_{\text{canonical}} \equiv Z^{-1}_{\text{canonical}} \int Dp \int Dp \;\; O\{\phi\}\; e^{-\beta H} \tag{3b}$$

$$Z_{\text{canonical}} \equiv \int Dp \int Dp \;\; e^{-\beta H} \tag{3c}$$

and

$$H = T + V \tag{3d}$$

The $\{p\}$ and $\{\phi\}$ are independent variables on the lattice.

Equations (2) and (3) define a "canonical ensemble", which represents the states of a system governed by a Hamiltonian H in contact with a heat reservoir at fixed temperature $\beta^{-1}$. This ensemble has kinetic energy $T\{p\}$ and potential energy $V\{\phi\}$. The isomorphism with a canonical ensemble is made complete by the identification

$$p_n = \frac{d\phi_n}{d\tau} \quad , \tag{4}$$

provided that a new "artificial dimension" $\tau$ is introduced. A Lagrangian formulation of field theory in d dimensions is thus mapped to a "Hamiltonian" formalism embedded in d discrete dimensions and one continuous ("artificial time") dimension. It will be seen that this artificial time coordinate corresponds roughly to the number of iterations in a numerical scheme.

A microcanonical ensemble[5,6] on the other hand describes a system in thermal isolation. Therefore the total "energy" of the system, $H[\{p\}, \{\phi\}]$ is constrained to a fixed value E, while the "temperature" $\beta^{-1}$ is defined to be the average kinetic energy of the system, suitably normalized. Each coordinate $\phi_n$ and momentum $p_n$ evolves in $\tau$ according to Hamilton's equations,

$$\frac{dp_n}{d\tau} = \frac{-\partial V[\phi]}{\partial \phi_n} \tag{5}$$

$$\frac{d\phi_n}{d\tau} = p_n \quad , \tag{6}$$

and expectation values of functionals $O[\{p\}, \{\phi\}]$ are determined by

$$\langle O \rangle_{micro} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_o^\tau O[\{p(\tau')\}, \{\phi(\tau')\}] \, d\tau' \tag{7}$$

where the coordinates $\{\phi(\tau)\}$ and momenta $\{p(\tau)\}$ are integrated along a trajectory in the 2N-dimensional phase space, using Eqs. (5) and (6). Therefore, the kinetic energy $T[p]$ and potential energy $V[\phi]$ are fluctuating quantities.

In order to establish the equivalence of $\langle O \rangle_{micro}$ and $\langle O \rangle_{canonical}$, it is necessary to assume that a hypothesis of ensemble theory known[13] as the "principle of equal weight" is satisfied. This principle assures us that the trajectories given by the solution of Eqs. (5) and (6) cover the (2N-1)-dimensional surface of constant energy E with equal density, and therefore that

$$\langle O \rangle_{micro} = Z_{micro}^{-1} \int Dp \int D\phi \; O[\{p\},\{\phi\}] \; \delta(H-E) \tag{8a}$$

where

$$Z_{micro} \equiv \int Dp \int D\phi \; \delta(H-E) \quad . \tag{8b}$$



In the thermodynamic limit, where N increases without bound, it can then be shown[2,3,14] that

$$\langle O \rangle_{micro} = \langle O \rangle_{canonical} + O(N^{-1} \langle O \rangle_{canonical}) \tag{9}$$

[It should be pointed out however that the subleading terms implicit in Eq. (9) become important whenever O takes the form of a variance (such as $\langle T - \langle T \rangle^2 \rangle$), for in cases like this the leading-order terms cancel].

## 3. Application to lattice gauge theories

It is useful at this juncture to apply the method of the microcanonical ensemble to a practical problem. In Refs. (5), (6) and (7), techniques for performing path integrals involving U(1), SU(2), and SU(3) gauge fields are explored in some detail. The results for U(1) gauge theory are briefly summarized here.

The standard formulation[15] of compact electrodynamics [i.e., U(1) lattice gauge theory] utilizes the action

$$\begin{aligned} S &= \beta V, \text{ with } \beta \equiv g_o^{-2} \\ V &\equiv \sum \mathrm{Re}(1 - U_{n,\mu} \, U_{n+\mu,\nu} \, U^{-1}_{n+\nu,\mu} U^{-1}_{n,\nu}) \\ U_{n,\mu} &\equiv \exp(i\phi_{n,\mu}) \end{aligned} \tag{10}$$

where $g_o$ is the bare lattice coupling constant and the sum defining V is over all elementary plaquettes on the lattice. The $\{\phi\}$ are real gauge fields associated with each link of the lattice; thus $U_{n,\mu}$ connects the lattice point n with its nearest neighbor in the direction $\mu$.

A calculation[5,6] of the average plaquette as a function of $\beta$ in this theory is now presented. The average plaquette is defined by the formula

$$P \equiv \left[2/d(d-1)\right] L^{-d} \langle V \rangle \tag{11}$$

on a hypercubic lattice in d (=4) dimensions whose side is L(=3) lattice sites. A comparison is made between the average plaquette calculated in the microcanonical ensemble and in the canonical ensemble (i.e., by standard[16,17] Monte Carlo methods). The average plaquette is calculated in the microcanonical ensemble by integrating numerically the equations of motion Eqs. (5) and (6), and evaluating the average plaquette and via Eq. (11). The inverse "temperature" $\beta^{-1}$ is determined by

$$\beta^{-1} = \frac{2}{N_{indep}} \langle T \rangle_{micro}, \tag{12}$$

where

$$N_{indep} = \frac{d-1}{d} N$$

$$= (d-1)L^d \tag{13}$$

with $N = dL^d$ the number of links in the lattice, and $N_{indep}$ is the number of <u>independent</u> degrees of freedom.

The reason that $N_{indep}$ is less than N is because there is a local gauge symmetry with no immediate physical relevance. General methods[18] exist for dealing with these redundant variables, familiar from classical mechanics as ignorable cyclic coordinates. One way to remove these ignorable coordinates is to impose constraints by choosing a gauge. Choices such as the axial gauge ($n_\mu A^\mu = 0$) or



the Lorentz gauge ($\partial_\mu A^\mu = 0$) result in a set of N/d constraints [cf. Eq. (13)] on a lattice of N links in d dimensions. The following course[5,6] seems more appropriate here.

By a suitable linear transformation from the variables $\{\phi\}$ to new variables $\{\xi\}$, the Hamiltonian equations of motion Eqs. (5) and (6) become:

$$\frac{d^2\xi_i}{d\tau^2} \equiv \ddot{\xi}_i = f_i(\{\xi\}), \quad i=1,2,\ldots N \tag{14a}$$

with

$$f_i(\{\xi\}) = 0, \quad N_{indep} < i \leq N \tag{14b}$$

It then follows that in solving Eqs. (5) and (6) if the initial condition $\dot{\phi}_{n,\mu} = 0$ at $\tau=0$ is imposed, the $\dot{\xi}_i$ for $N_{indep} < i \leq N$ will equal zero for all $\tau$. As a consequence in the average in Eq. (12) the correct divisor is $N_{indep}$ and not N. This procedure is analogous to determining the temperature of a system of particles by measuring the average kinetic energy per particle in the rest frame of the system (equivalent to imposing d constraints).

The results of the computation in each of the two ensembles are now presented. In the microcanonical-ensemble calculation the ordinary differential equations Eqs. (5) and (6) are integrated by the Runge-Kutta method with step size $\Delta\tau = 0.01$ (step sizes as large as $\Delta\tau = 0.1$ still lead[5,6] to energy conservation to better than one part in $10^4$). At genesis ($\tau=0$) each of the $\{\phi\}$ is chosen randomly between 0 and $2\pi$, and each of the $\{p\}$ is set to zero (for reasons described above). Expectation values are obtained as an

average over $\tau = 2{,}000\ \Delta\tau$ (i.e., by using 2,000 consecutive configurations).

After each calculation (or set of 2000 "measurements") was completed, the value of E (and hence $\beta$) was altered by multiplying all of the $\{p\}$ by the same factor. This operation effectively heats [cools] the system if the factor is greater than [less than] unity. The Runge-Kutta algorithm is then applied to step the system forward from $\tau$ to $\tau + \Delta\tau$. By a proper choice of this heating/cooling factor after each step the value of $\beta$ can be easily adjusted to a given value with arbitrary accuracy after enough steps. The heating/cooling cycle is terminated after 1000 $\Delta\tau$ and the system was allowed to equilibrate for 3000 $\Delta\tau$ before more measurements were taken. On each such energy shell the system has a unique value of $\langle V\rangle_{micro}$ and hence of $\langle T\rangle_{micro}$ and $\beta$. Note that this heating/cooling procedure conserves the vanishing of $\dot{\xi}$ for $N_{indep} < i \leq N$.

In the canonical-ensemble calculation the standard algorithm[16] of Metropolis, et. al. is used for the Monte Carlo simulation. At each $\beta$, equilibration for 200 iterations is allowed after which the average plaquette is measured for 2000 iterations.

Figure 1 displays the value of the average plaquette as a function of $\beta$ for both ensembles. The agreement between the two calculations is excellent, and the amount of computer time required for each calculation is roughly the same (although no attempts at optimization were made).



## 4. Generalization of the microcanonical method

### a. Hybrid stochastic method

It has been suggested[10] that a combination of the ideas of microcanonical simulation with the notion of "stochastic quantization",[19] sometimes called a Langevin method, can lead to improvements over both methods. In the stochastic method a gaussian white noise function $\eta_i(s)$ is introduced by

$$\frac{d\phi_i}{ds} = -\frac{\partial V\{\phi\}}{\partial \phi_i} + \eta_i(s) \tag{15a}$$

with[19]

$$\langle \eta_i(s')\ \eta_j(s)\rangle_{ens} = 2\beta^{-1}\ \delta_{ij}\,\delta(s'-s) \tag{15b}$$

Expectation values are calculated by

$$\langle O\{\phi\}\rangle_{ens} = \overline{O\{\phi\}} \tag{16a}$$

$$= \lim_{s\to\infty} \frac{1}{s} \int_0^s ds'\ O\{\phi(s')\} \tag{16b}$$

where the brackets $\langle\ldots\rangle_{ens}$ denote an "ensemble" average over an infinite number of thermodynamically equivalent systems. As the Langevin equation has explicit noise (generated by $\eta_i(s)$) it is ergodic by construction, and therefore Eqs. (16) hold.

Compare Eq. (15a) with the corresponding microcanonical equation of motion:

$$\frac{dp_i}{d\tau} = \frac{d^2\phi_i}{d\tau^2} = -\frac{\partial V\{\phi\}}{\partial \phi_i} \tag{17}$$

It is difficult to miss the similarity between the two. In fact, if ergodicity and a few general properties of a microcanonical ensemble are assumed, the stochastic quantization procedure can be "derived" as a consequence of the microcanonical ensemble.[12]

Consider the (artificial) time correlation function of two momenta in the microcanonical ensemble:

$$\langle p_i(\tau')\ p_j(\tau)\rangle_{ens} = \beta^{-1}\ \delta_{ij}\ C(\tau-\tau') \tag{18}$$

where the equality of the ensemble and microcanonical averages (ergodicity) is assumed. Given that a "correlation time" $\epsilon$ can be defined by

$$\int_{-\infty}^{\infty} d\tau\ \ C(\tau) = 2\epsilon \tag{19}$$

it is assumed that $C(\tau)$ is zero for $|\tau|$ much greater than $\epsilon$. thus if $C(\tau)$ is measured over time scales much greater than $\epsilon$ it will be observed that

$$C(\tau)\ d\tau \rightarrow 2\epsilon\ \delta(\tau)\ d\tau \tag{20}$$

A pedagogically convenient (though overly simplified) model for $C(\tau)$ is:

$$C(\tau) = \exp(-|\tau|/\epsilon) \tag{21}$$

This model is suggested for purposes of illustration only, and is not needed for the following discussion.

Next consider Eq. (17), which defines the trajectories $\{p(\tau),\ \phi(\tau)\}$ in the microcanonical ensemble. If this equation is integrated from $\tau-\epsilon$ to $\tau$ the result can be written

$$p_i(\tau) = \frac{d\phi_i(\tau)}{d\tau}$$

$$= -\int_{\tau-\epsilon}^{\tau} \frac{\partial V}{\partial \phi_i}\ d\tau' + p_i(\tau-\epsilon) \tag{22}$$

During the interval $\epsilon$, the fields $\{p\}$ become essentially independent of their initial values, and so $p_i(\tau)$ is uncorrelated with $p_i(\tau-\epsilon)$.



This process occurs in a smooth and analytic fashion, so if the ensemble is observed over time scales large compared with $\epsilon$, it is reasonable to expand the integrand in Eq.(22) for small $\epsilon$. The result is Eqs. (15) with the redefinitions

$$s = \epsilon\tau \qquad \eta(s) = \epsilon^{-1}\ p(\tau-\epsilon) \tag{23}$$

and with $\epsilon^2$ corrections dropped. Thus it is seen that the stochastic quantization formalism is essentially a <u>consequence</u> of ergodic microcanonical field theory.

The above discussion should clarify the similarities and differences between the microcanonical and Langevin schemes. In terms of computational efficiency, the following attributes of the two methods are obvious:[10,11] 1) Microcanonical dynamics follows the classical equations of motion of the system, so it is as efficient as possible in exploring the important regions of phase space. Also, its time step is typically larger (by a factor $\epsilon^{-1}$) than in the Langevin scheme, so it moves along its trajectories rapidly. Of all schemes, the microcanonical one seems best equipped to show any physics which hinges upon the effective integration of the "soft" modes of the system. However, it may not be ergodic, and thus may not explore all regions of phase space equally well. 2) The Langevin scheme, on the other hand, has explicit noise, and so is ergodic by construction. However, it samples the phase space of the system very slowly in many cases because $\phi(\tau)$ executes a random walk which, if the noise term dominates the drift term, fills space at a rate proportional to $\sqrt{N}$, where N is the the number of time steps.

This comparison suggests that the best of all possible worlds can be achieved by adopting a hybrid scheme[10] which combines the best features of both approaches. Consider a simple discretization of Eqs. (15) and (17):

$$\phi_i(\tau+\Delta\tau) = \phi_i(\tau) + (\Delta\tau)\, V_i - \frac{1}{2}(\Delta\tau)^2 \frac{\partial V[\phi]}{\partial \phi i} \qquad (24a)$$

where

$$V_i = \begin{cases} \eta_i & \text{with probability } p(\Delta\tau) \\ \dfrac{\phi_i(\tau+\Delta\tau) - \phi_i(\tau-\Delta\tau)}{2\,\cdot\,\Delta\tau} & \text{otherwise} \end{cases} \qquad (24b)$$

This "hybrid" scheme updates the entire system either by the Langevin method (with $p.\Delta\tau$) or the microcanonical methods (with probability $1 - p.\Delta\tau$). The best choice[11] for p seems to be twice the frequency of the slowest mode in the system (implying of course that the hybrid scheme really is better than either a pure microcanonical method or pure Langevin dynamics). The hybrid scheme has also been applied to do a calculation of finite-temperature behavior in QCD.[11]

4b. "Canonical molecular dynamics" methods

One feature of the microcanonical method is that the "temperature" β (related to the bare coupling constant in a lattice gauge theory by $\beta=g_o^{-2}$) is a calculated, "output" parameter. As pointed out above, and in the original work,[5,6] β can be adjusted to arbitrary accuracy by a "heating/cooling" cycle where all the momenta of the system are repeatedly rescaled by a common factor following each update. A more direct approach[20] is possible however, which is often called a "demon" method, after a similar



idea used for the Ising model.[9]

Consider the effects of modifying the Eqs. (2) and (3) by allowing a "dynamical mass" or demon s,

$$H_{demon} = \sum_{i=1}^{N} \frac{p_i^2}{2s^2} + V[\phi] + \frac{N+1}{\beta} \ln s + \frac{1}{2} p_s^2 \qquad (25)$$

Calculate the partition function for the demon system in the microcanonical ensemble:

$$Z_{demon} = \int dp_s \int ds \int Dp\, D\phi\ \ \delta(H-E) \qquad (26)$$

Rescale $\{p\} \to \{p/s\}$, then do the integral over s using the delta function and do the $p_s$ gaussian integral trivially to find

$$Z_{demon} = Z_{micro} = \int Dp\, D\phi\ \ \exp(-\beta H) \qquad (27)$$

where H is given by Eq. (3d). Thus it is seen that the "canonical molecular dynamics" or "demon" method reproduces the canonical ensemble. This method has been tested successfully on the two-dimensional planar spin model.[11] Useful features of this method include the facts that 1) β can be chosen as an input variable. 2) Finite system effects are suppressed. 3) Equilibration can be monitored closely via $\langle p_s^2/2\rangle = 2\beta^{-1}$.

5. Microcanonical simulation of fermionic systems

As suggested in the initial work[5,6] the microcanonical ensemble can be useful for fermionic simulations as well. Typically calculations involving fermions can be reduced[3] to the simulation of an effective action $S_F$:

$$S_F[\phi] = S_G[\phi] - \ln \det M[\phi] \qquad (28)$$

where $S_G\{\phi\}$ is the pure gauge part of the action, and $M\{\phi\}$ is a large real (usually local) matrix which arises in the fermionic action. The naive microcanonical equations of motion are[5]

$$\ddot{\phi}_i = - \frac{\partial S_G}{\partial \phi_i} + \mathrm{Tr}\left[M^{-1} \frac{\partial M}{\partial \phi_i}\right] . \tag{29}$$

which are difficult to integrate because of the need to invert the matrix M repeatedly (for a typical calculation, M has at least as many elements as sites on the lattice). Conventional Monte Carlo simulation does no better, for it requires the re-evaluation of the determinant in Eq. (29) at each step (to evaluate a determinant takes roughly one-third the time matrix inversion does). Some improvement over these methods can be obtained by using the method[7] of Polonyi and Wyld. Their method uses the Hamiltonian

$$H_{PW} = \sum_{m,n} P_m^* M^{-1}\{\phi\} P_n + w^2 \sum_n Q_n^* Q_n + \frac{1}{2} \sum_i p_i^2 + S_G\{\phi\} \tag{30}$$

where the $\{P\}$ and $\{Q\}$ are introduced to simulate the fermionic part of the action. This follows because of the fact that in the canonical ensemble

$$\int DP \; DQ \; Dp e^{-H_{PW}} = e^{-S_F\{\phi\}} \tag{31}$$

apart from an irrelevant constant factor. The microcanonical equations of motion which follow from Eq. (30) can be written in th form

$$\sum_n \frac{d}{d\tau}\left[M_{mn}\{\phi\} \frac{dQ_n}{d\tau}\right] = w^2 Q_m \tag{32a}$$

$$\frac{d^2\phi_i}{d\tau^2} = - \frac{\partial S_G\{\phi\}}{\partial \phi_i} + \sum_{m,n} Q_m^* \frac{\partial M_{mn}}{\partial \phi_i} Q_n \tag{32b}$$



The simplification occurs because the solution of the linear system Eq. (32a) is slightly easier than the matrix inversion implied in Eq.(29). The point is that although one can formally solve a linear system

$$Ax = y \tag{33}$$

for the vector x (given the matrix A and vector y) by the substitution

$$x = A^{-1}y \tag{34}$$

that this is not the most efficient method computationally (conjugate gradient algorithms are often recommended for the direct solution of Eq. (33)).

This microcanonical method for fermions appears[7] to perform well in studies of the two-dimensional Schwinger model as well as for four-dimensionl QCD with fermions. Various improvements have also been proposed.[11] In general it seems to perform at least as well as other algorithms[21] currently applied; however, given the enormous amounts of computer time involved, even a slight improvement is important (ten percent of a very large number is still a large number). Unfortunately a really satisfactory method for incorporating fermions has yet to be devised.

## 6. Summary

Various methods of applying the method of the microcanonical ensemble to lattice gauge theories have been discussed. Still, the art of numerical simulation of quantum field theory is in its infancy, and the future will no doubt bring with it more powerful algorithms and faster machines upon which they may be applied. Progress in both these areas shall certainly continue.

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FIGURE CAPTION

Figure 1 Microcanonical ensemble calculation (dots) and Monte Carlo calculation (circles) of the average plaquette P versus β for a U(1) gauge system on a $3^4$ lattice.