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Microcanonical Technology for Lattice Gauge Theory* †

David J.E. Callaway
Department of Physics
The Rockefeller University
1230 York Avenue
New York, New York 10021-6399

Abstract

Various techniques for the application of the microcanonical formulation of lattice gauge theory are discussed.

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† Dedicated to the memory of Aness Rahman

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 he updated in a single pass because each link interacts with its neighbors, and so a simultaneous update of link and neighhor 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

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

where

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

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

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

where

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

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

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 β^{-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" τ 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" β^{-1} is defined to be the average kinetic energy of the system, suitably normalized. Each coordinate ϕ_n and momentum p_n evolves in τ 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

$$\langle O \rangle_{micro} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau O[\{p(\tau')\}, \{\phi(\tau')\}]\, d\tau' \tag{7}$$

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

$$S = \beta V, \text{ with } \beta \equiv g_o^{-2}$$

$$V \equiv \sum \mathrm{Re}(1 - U_{n,\mu}\, U_{n+\mu,\nu}\, U^{-1}_{n+\nu,\mu} U^{-1}_{n,\nu})$$

$$U_{n,\mu} \equiv \exp(i\phi_{n,\mu}) \tag{10}$$

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 μ.

A calculation[5,6] of the average plaquette as a function of β 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" β^{-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 τ. 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 2π, 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 β) 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 τ to $\tau + \Delta\tau$. By a proper choice of this heating/cooling factor after each step the value of β 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 β. 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 β, 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 β 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. Variations on the original method

a) Measuring the coupling constants

Rather than determining the coupling constants (like β in the above example) from the average kinetic energy $\langle T\rangle$ it is possible to extract them directly from measurements over coordinates ϕ. Various identities can be derived in the canonical ensemble and then related to the corresponding microcanonical quantities. In a gauge theory, these "loop equations" identities are derived by using the gauge invariance of the integration measure. Consider the above example of a U(1) gauge theory. If $O(\phi)$ denotes a 2π-periodic function of the ϕ_i, then

$$\int_{-\pi}^{\pi} d\phi_i \quad \frac{d}{d\phi_i} \quad [O(\phi)\, e^{-S(\phi)}] = 0 \tag{15}$$

holds identically. A convenient choice is

$$O(\phi) = \frac{d}{d\phi_i} V \tag{16}$$

Then Eq. (15) implies that

$$\beta = \frac{\left\langle \dfrac{d^2 V}{d\phi_i^2} \right\rangle}{\left\langle \left(\dfrac{d V}{d\phi_i} \right)^2 \right\rangle} \tag{17}$$

In practice, quantities are averaged over all ϕ_i so as to improve statistics. Thus β can be determined for any given initial values of the momenta p_i, and special initial conditions are not needed.

The constant β can be chosen via the "heating/cooling" procedure described above, or by updating portions of the system by other methods. The case where a small part of the system is updated by a standard Monte Carlo procedures but the majority of the degrees of freedom in the theory are microcanonical can be [6] referred to as maintaining loose contact with a heat bath. Other methods of combining, e.g., microcanonical and Langevin approaches have also been considered (see, [10]).

b) Constraint dynamics

The microcanonical formalism can be implemented in an entirely different fashion, using constraints and Lagrange multipliers. As an example consider again the U(1) lattice gauge theory, whose Haar measure can be cast in terms of a constraint:

$$\int dU = \int_{-1}^{1} dx \int_{-1}^{1} dy \;\; \delta(x^2 + y^2 - 1) \tag{18}$$

where

$$x \equiv \mathrm{Re}(U) \tag{19a}$$

$$y \equiv \mathrm{Im}(U) \tag{19b}$$

The corresponding microcanonical theory uses the variables $U_{n,\mu}$ directly as the canonical variables. The constraint $|U_{n,\mu}|^2 = 1$ is implemented by the method of Lagrange multipliers A constraint potential

$$V_c = \sum_{n\mu} \lambda(U_{n\mu}) \left[1 - |U_{n,\mu}|^2\right] \tag{20}$$

(where λ is the Lagrange multiplier) is added to the potential V of Eq. (10). The implied set of microcanonical differential equations can be integrated by the following procedure. Call the force generated on link $U_{n,\mu}$ only by V (and <u>not</u> including the force of constraint) $F_{n,\mu}(\tau)$:

$$F_{n,\mu} = -\frac{\partial V}{\partial U_{n,\mu}} \tag{21}$$

Given the values of the coordinates $U_{n,\mu}(\tau)$ and their velocities $\dot{U}_{n,\mu}(\tau) \equiv d\, U_{n,\mu}(\tau)/d\tau$ the incomplete new coordinate is formed (here h is the step size):

$$W_{n,\mu}(\tau+h) = U_{n,\mu}(\tau) + h\, \dot{U}_{n,\mu}(\tau) + \frac{1}{2} h^2 F_{n,\mu}(\tau) \tag{22}$$

The new coordinate $U_{n,\mu}(\tau+h)$ is then given by

$$U_{n,\mu}(\tau+h) = W_{n,\mu}(\tau+h) + \frac{1}{2} \lambda(U,\tau)\, U^{*}_{n,\mu}(\tau) \tag{23}$$

[In equation (23), $U^{*}_{n,\mu}(\tau)$ comes from the derivative of the constraint potential]. The value of $\lambda(U,\tau)$ is determined via the quadratic equation resulting from the constraint condition .

$$|U_{n,\mu}(\tau+h)|^2 = 1 \tag{24}$$

assuming that this constraint holds at time τ. The update is then completed by calculating $\dot{U}_{n,\mu}(\tau+h)$. First, a new set of forces F $F_{n,\mu}(\tau+h)$ is calculated from $U_{n,\mu}(\tau+h)$. From these forces the incomplete new velocity is constructed:

$$\eta_{n,\mu}(\tau+h) \equiv \dot{U}_{n,\mu}(\tau) + \frac{1}{2} \left[F_{n,\mu}(\tau) + \lambda(U,\tau)\, U_{n,\mu}(\tau) + F_{n,\mu}(\tau+h)\right] \tag{25}$$

whence $\dot{U}_{n,\mu}(\tau+h)$ is given by

$$\dot{U}_{n,\mu}(\tau+h) = \eta(\tau+h) + \mu\, h\, U_{n,\mu}(\tau+h) \qquad (26)$$

The new constraint parameter $\mu(\tau)$ is determined by the τ-derivative of the constraint $|U_{n,\mu}|^2 = 1$:

$$\mathrm{Re}\,[\dot{U}_{n,\mu}(\tau+h)\, U^{*}_{n,\mu}(\tau+h)] = 0 \qquad (27)$$

This completes the update of the system. It can therefore be seen that there are several ways to do a microcanonical simulation of a U(1) gauge theory [see [6] for discussions of techniques for SU(2) and SU(3)].

5. Summary

Various methods of using the microcanonical approach to lattice gauge theory have been discussed. Nevertheless, the art of such simulations is still in its infancy, and no doubt progress will continue.

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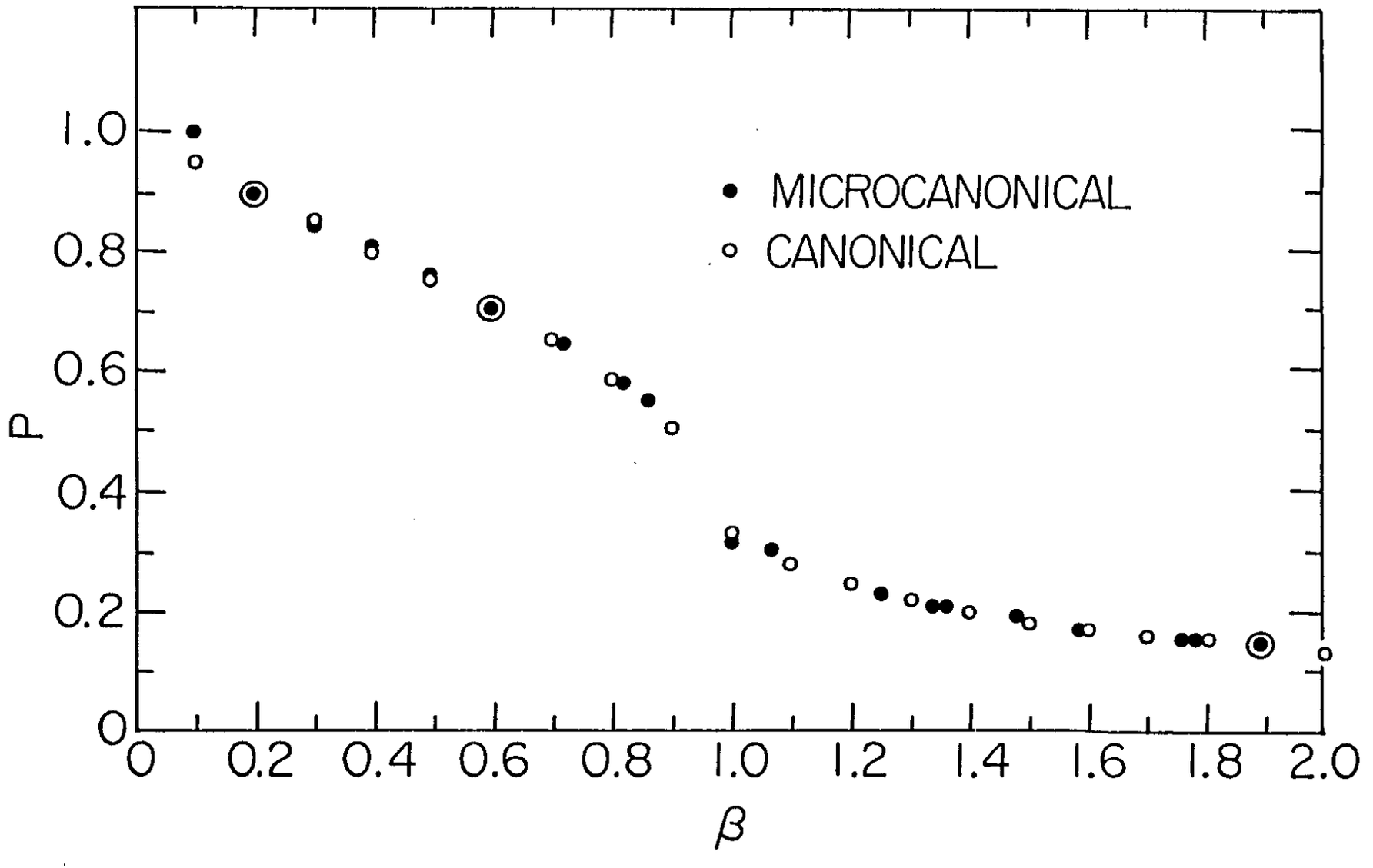
FIGURE CAPTION

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.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0.8
0.6
0.4
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p
0
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0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
β
MICROCANONICAL
CANONICAL