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Microcanonical Ensemble Formulation of Lattice Gauge Theory

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A new formulation of lattice gauge theory without explicit path integrals or sums is obtained by using the microcanonical ensemble of statistical mechanics. Expectation values in the new formalism are calculated by solving a large set of coupled, nonlinear, ordinary differential equations. The average plaquette for compact electrodynamics calculated in this fashion agrees with standard Monte Carlo results. Possible advantages of the microcanonical method in applications to fermionic systems are discussed.

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The formulation of gauge theories on a lattice has led to great progress in understanding relativistic quantum field theory. The use of the lattice spacing as an ultraviolet cutoff allows the calculation of relevant physical quantities without resorting to perturbation theory, which by itself is severely limited in computational possibilities.

In the usual approach[1] to lattice gauge theory the central assumption is that expectation values of functionals $\mathcal{O}$ of fields $\{\varphi\}$ on a finite Euclidean lattice can give physically meaningful results without having to go to the continuum limit. With use of an action $S\{\varphi\}$, with a finite number N of fields $\{\varphi\}$ and suitable boundary conditions, such expectation values are defined by

$$\langle \mathcal{O} \rangle_{\text{lattice}} \equiv Z^{-1} \int \mathfrak{D}\varphi\, \mathcal{O}\{\varphi\} e^{-S\{\varphi\}},$$
$$Z \equiv \int \mathfrak{D}\varphi\, e^{-S\{\varphi\}}, \qquad (1)$$
$$\int \mathfrak{D}\varphi \equiv \int d\varphi_1 \int d\varphi_2 \cdots \int d\varphi_N.$$

The continuum limit is obtained as N increases without bound and the lattice spacing approaches zero. As discussed below, the standard lattice path-integral formalism, Eqs. (1), is isomorphic to a *canonical ensemble*, familiar from classical statistical mechanics.

We propose an alternative formulation for lattice gauge theory. In this new formalism (hereafter referred to as the *microcanonical ensemble*)

an explicit path integral or sum does not appear. Instead expectation values are calculated by solving a set of N coupled, nonlinear, second-order, ordinary differential equations.

Our results show that for $N \gtrsim 100$ the two ensembles give essentially identical results for the average plaquette in a U(1) gauge theory. Furthermore, we believe that in certain instances the microcanonical method may be superior to the conventional path-integral method, for which Monte Carlo techniques are traditionally used[2] to perform the integrations. The two methods are now compared by use of a particular example.

The standard formulation[1,3] of compact electrodynamics [i.e., a lattice U(1) gauge theory] utilizes the action

$$S=\beta V \text{ with } \beta=1/g_0^2, \tag{2a}$$

$$V\equiv\sum \mathrm{Re}(1-U_{n,\mu}U_{n+\mu,\nu}U_{n+\nu,\mu}^{\dagger}U_{n,\nu}^{\dagger}) \tag{2b}$$

$$U_{n,\mu}=\exp(i\varphi_{n,\mu}), \tag{2c}$$

where g_0^2 is the bare lattice coupling constant and the sum defining V is over all elementary plaquettes in d dimensions. The $\{\varphi\}$ are real gauge fields associated with each link of the lattice; the link $U_{n,\mu}$ connects the lattice point n to its nearest neighbor in the direction μ.

Any quantity independent of all $\{\varphi\}$ can be added to the action $S\{\varphi\}$ without affecting the expectation value of any functional of the $\{\varphi\}$. Hence, it follows that

$$\begin{aligned}&\langle\mathcal{O}\rangle_{\text{lattice}}=\langle\mathcal{O}\rangle_{\text{canon}}\equiv Z_{\text{canon}}^{-1}\int\mathfrak{D}\varphi\int\mathfrak{D}p\,e^{-\beta H}\mathcal{O}\{\varphi\},\\ &Z_{\text{canon}}\equiv\int\mathfrak{D}\varphi\int\mathfrak{D}p\,e^{-\beta H},\\ &\int\mathfrak{D}p\equiv\int dp_1\int dp_2\cdots\int dp_N,\\ &H\equiv T+V,\quad T\equiv\tfrac{1}{2}\sum_{i=1}^{N}p_i^2.\end{aligned} \tag{3}$$

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

An obvious isomorphism with classical statistical mechanics arises on making the identification

$$d\varphi_{n,\mu}/d\tau=p_{n,\mu} \tag{4}$$

if we introduce a new "dimension" or artificial variable τ. A Lagrangian formulation of a Euclidean quantum field theory embedded in d discrete dimensions [Eqs. (1) and (2)] is thus mapped to a "Hamiltonian" formalism[4] embedded in d discrete dimensions and one continuous dimension.

Note that H is invariant under local gauge transformations

$$U_{n,\mu}+W_nU_{n,\mu}W_{n+\mu}^{\dagger} \tag{5}$$

provided that the W_n, elements of the U(1) gauge group, are independent of τ.

Equations (2) and (3) define a canonical ensemble with kinetic energy T, potential energy V, and temperature β^{-1}. This ensemble represents the states of a system (governed by a Hamiltonian H) in contact with a heat bath at fixed temperature β^{-1}.

A microcanonical ensemble, on the other hand, describes a system in thermal isolation and hence the "energy" $H[\{\varphi\},\{p\}]$ of the system is constrained to be a fixed value E, while the "temperature" β^{-1} is defined to be the average kinetic energy (suitably normalized).[5] Each coordinate evolves in τ according to Hamilton's equations,

$$\frac{d^2\varphi_{n,\mu}}{d\tau^2}=\dot{p}_{n,\mu}=-\frac{\partial V\{\varphi\}}{\partial\varphi_{n,\mu}}. \tag{6}$$

Formally, expectation values in the microcanonical ensemble are written as

$$\langle\mathcal{O}\rangle_{\text{micro}}\equiv Z_{\text{micro}}^{-1}\int_{H=E}\mathfrak{D}\varphi\mathfrak{D}p\,\mathcal{O}[\{\varphi\},\{p\}], \tag{7a}$$

with

$$Z_{\text{micro}}\equiv\int_{H=E}\mathfrak{D}\varphi\,\mathfrak{D}p. \tag{7b}$$

The integrals in Eqs. (7) are over the $(2N-1)$-dimensional hypersurface of constant "energy," $H[\{\varphi\},\{p\}]=E$.

The expectation value of any functional of the $\{\varphi\}$ and $\{p\}$ can be calculated by use of the $\{\varphi\}$ and $\{p\}$ generated along the trajectory given by the solution of Eqs. (6) in the $2N$-dimensional phase space $\{\varphi,p\}$. Any expectation value is thus given by

$$\langle\mathcal{O}\rangle_{\text{micro}}=\lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau}\mathcal{O}\{\varphi(\tau'),p(\tau')\}d\tau', \tag{8}$$

and is a unique function of E.

The equivalence of Eqs. (7) and (8) follows from a vital assumption of ensemble theory known as the principle of equal weight.[6] This principle assures us that for a given E, the trajectories given by the solution of Eqs. (6) cover the $(2N-1)$-dimensional constant-energy surface in phase space $\{\varphi,p\}$ with equal density. The additional assumption that all expectation values of a physical system can be computed in either ensemble is discussed and partially proven by Fisher,[7] Griffith,[7] Van der Linden,[7] and Lebowitz, Percus,

and Verlet.[8]

The average kinetic energy $\langle T\rangle$ which defines the analog "temperature" (i.e., the bare lattice coupling constant) along a trajectory is given by

$$g_0^2=\beta^{-1}=(2/N_{\text{indep}})\langle T\rangle_{\text{micro}}. \tag{9}$$

The significance of N_{indep} is discussed below. Another quantity of interest is the average action,

$$\langle S\rangle_{\text{micro}}=\beta\langle V\rangle_{\text{micro}}. \tag{10}$$

As regards N_{indep}, recall that in a lattice gauge theory there is a local gauge symmetry with no immediate physical relevance. Because of this symmetry there are only $N_{\text{indep}}<N$ linearly independent variables among the $\{\varphi\}$. In the thermodynamic limit ($N\to\infty$) the number of linearly independent variables in d dimensions for the U(1) gauge theory is

$$N_{\text{indep}}=[(d-1)/d]N=(d-1)L^d, \tag{11}$$

for a hypercube with L lattice sites along each side.

General methods exist[9] for dealing with 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 on a lattice of N links in d dimensions. The following course seems more appropriate here.

By a suitable linear transformation on the variables $\varphi_{n,\mu}$ to new variables ξ_i, Eqs. (6) become

$$\ddot{\xi}_i\equiv d^2\xi_i/d\tau^2=f_i(\{\xi\}),\quad i=1,2,\ldots N, \tag{12}$$

with

$$f_i(\{\xi\})=0,\quad N_{\text{indep}}<i\leq N. \tag{13}$$

It then follows that in solving Eqs. (6) if the initial condition $\dot{\varphi}_{n,\mu}=0$ at $\tau=0$ is imposed, the $\dot{\xi}_i$ for $N_{\text{indep}}<i\leq N$ will equal zero for all τ. As a consequence in the average in Eq. (9) 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 of each particle in the rest frame of the system (equivalent to imposing d constraints).

The results of numerical calculations performed in each of the two ensembles are now compared for the U(1) lattice gauge theory. These calculations were performed in four Euclidean dimensions on a periodic lattice of size 3^4. In each case, the average plaquette,

$$P\equiv[2/d(d-1)]L^{-d}\langle V\rangle, \tag{14}$$

is plotted as a function of β.

In the microcanonical ensemble calculation the ordinary differential equations Eq. (6) are solved by the Runge-Kutta method with step size $\Delta\tau=0.01$. At $\tau=0$ each $\varphi_{n,\mu}$ is chosen randomly between zero and 2π, and each $\dot{\varphi}_{n,\mu}$ is set to zero (for reasons mentioned above). Expectation values are obtained as an average over $\tau=2000\Delta\tau$ (i.e., using 2000 consecutive configurations).[10]

After each calculation (or set of 2000 "measurements") is completed, the value of E is 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 $\tau+\Delta\tau$, and the heating/cooling process is repeated. This heating/cooling cycle is terminated after $1000\Delta\tau$ and the system is allowed to follow its trajectory on the new energy shell for $3000\Delta\tau$ to allow the system to equilibrate before more measurements are taken. On each such energy shell in a state of equilibrium the system has a unique value of $\langle T\rangle_{\text{micro}}$ and hence of $\langle V\rangle_{\text{micro}}$ and β [cf. Eq. (9)]. Note that the heating/cooling procedure conserves the vanishing of $\dot{\xi}_i$ for $i>N_{\text{indep}}$.

In the calculation of the canonical average the standard Metropolis[11] Monte Carlo algorithm is used. At each β, equilibration for 200 iterations is allowed after which the average plaquette is measured for 2000 iterations. Further details are given elsewhere.[12]

In Fig. 1 values of the average plaquette as a function of β are displayed for both ensembles. The agreement between the two sets of results is excellent. The amount of computer time required for each calculation is roughly the same.

The microcanonical ensemble method appears particularly promising for systems involving fermions. Such systems are governed by an action which (after the fermionic degrees of freedom are integrated out) is of the form

$$S=\beta_1 S_{\text{gauge}}+\beta_2 \ln \operatorname{Det} \underline{A}, \tag{15}$$

where β_1, β_2 are constants, S_{gauge} is the action for a pure gauge system [such as the action for compact electrodynamics, Eq. (2)], and $\underline{A}$ is a Hermitian matrix arising from the interaction of gauge fields with fermions.

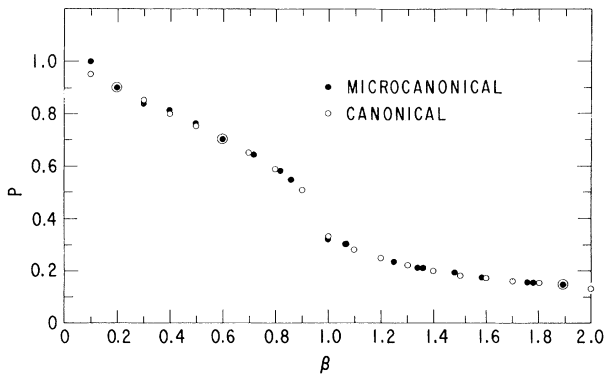

FIG. 1. Microcanonical ensemble calculation (dots) and Monte Carlo calculation (circles) of the average plaquette P vs β for a U(1) gauge system on a 3^4-site lattice.

In this case the microcanonical approach leads to an equation of "motion,"

$$\ddot{\varphi}_{n,\mu} = -\frac{\partial S_{\text{gauge}}}{\partial \varphi_{n,\mu}} - \frac{\beta_2}{\beta_1} \sum_{ij}{}' (\underline{A}^{-1})_{ij} \frac{\partial A_{ij}}{\varphi_{n,\mu}}, \qquad (16)$$

for the case of fermions interacting with a U(1) gauge field. The Metropolis routine applied directly to the action Eq. (15) requires the determinant to be reevaluated after *each link* is tentatively updated. However, to update the *entire lattice* with the microcanonical approach [via Eq. (16)] and, e.g., a predictor-corrector algorithm, $\underline{A}^{-1}$ must be calculated once and Det $\underline{A}$ is obtained at the same time.[13] Of course $\underline{A}^{-1}$ is needed already for calculating several quantities of interest (e.g., propagators). Work along these lines on fermionic systems is in progress.

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