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A Statistical Mechanics View of Quantum Chromodynamics: Lattice Gauge Theory[1]

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Recent developments in lattice gauge theory are discussed from a statistical mechanics viewpoint. The basic physics problems of quantum chromodynamics (QCD) are reviewed for an audience of critical phenomena theorists. The idea of local gauge symmetry and color, the connection between statistical mechanics and field theory, asymptotic freedom and the continuum limit of lattice gauge theories, and the order parameters (confinement and chiral symmetry) of QCD are reviewed. Then recent developments in the field are discussed. These include the proof of confinement in the lattice theory, numerical evidence for confinement in the continuum limit of lattice gauge theory, and perturbative improvement programs for lattice actions. Next, we turn to the new challenges facing the subject. These include the need for a better understanding of the lattice Dirac equation and recent progress in the development of numerical methods for fermions (the pseudofermion stochastic algorithm and the microcanonical, molecular dynamics equation of motion approach). Finally, some of the applications of lattice gauge theory to QCD spectrum calculations and the thermodynamics of QCD will be discussed and a few remarks concerning future directions of the field will be made.

KEY WORDS: Lattice gauge theory; quantum chromodynamics; confinement; computer simulations.

1. LATTICE GAUGE THEORY AND QUANTUM CHROMODYNAMICS BACKGROUND

1.1. Local Color Gauge Invariance

The basic constructive dynamical principle of QCD is local color symmetry. Following Yang and Mills[(1)] in concept but in a different context, we

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consider quark fields $\psi_i(x)$ having a color $SU(3)$ index i. To think about color $SU(3)$ as a local symmetry, we imagine independent color frames of reference at each point of space-time. The theory's action is required to be invariant under local rotations of these color frames. An $SU(3)$ rotation matrix $U_p(x, y)$ will describe the relative orientation of local frames at points x and y, when they are parallel-transported along the path P. It is convenient to introduce an operator $G_\theta(x)$ which rotates the local frames of reference by the space-time-dependent angle $\theta(x)$, $G_\theta(x) = \exp[i\lambda^\alpha\theta_\alpha(x)/2]$. From their geometric meaning the variables $U_p(x, y)$ transform under the local rotation operator G as

$$U_p(x, y) \rightarrow G_\theta(x) U_p(x, y) G_\theta^{-1}(y) \tag{1.1}$$

The $U_p(x, y)$ will be the basic degrees of freedom of the gauge theory and the action of the theory will be postulated to be invariant under the local color symmetry operations Eq. (1.1). This means that the action should be constructed from the quantities tr $U_c(x)$, where c denotes a closed contour.

To be more specific we parametrize $U_p(x, y)$ for infinitesimally nearby points x and y as

$$U_\mu(x) = \exp(igA_\mu^\alpha \lambda^\alpha\, dx_\mu/2) \tag{1.2}$$

where λ^α are the eight Gell-Mann matrices of color $SU(3)$ and A_μ^α can be identified, following the pioneering work of Yang and Mills[1] as the eight gluon fields. The rotation matrices for finite paths are then constructed,

$$U_p(x, y) = P \exp\left(ig \int_p A_\mu^\alpha \lambda^\alpha\, dx_\mu/2\right) \tag{1.3}$$

where P denotes a path-ordered product and the locally gauge invariant quantity used for the construction of the action is

$$W(c) = \operatorname{tr} P \exp\left(ig \oint_c A_\mu^\alpha \lambda^\alpha\, dx_\mu/2\right) \tag{1.4}$$

From this explicitly gauge-invariant perspective in which $W(c)$ is the basic variable of the theory, one can study gauge theories as the theory of chiral fields defined on a base space consisting of all closed contours c. A. M. Polyakov[2] has pioneered this viewpoint and has sought closed solutions, in analogy to the solution of integrable two-dimensional chiral models, of pure gauge theories. Although this viewpoint has yet to attain its goal, it has led to new developments such as interesting connections to the theory of strings,[3] developed some time ago for high-energy phenomenology.

Lattice gauge theory, as invented by A. M. Polyakov[2] and independently by K. G. Wilson[4] and introduced even earlier for simple gauge groups in a statistical mechanics setting by F. Wegner,[5] begins with precisely this viewpoint. However, to make the base space of all contours enumerable and to make useful, local actions, it replaces space-time by a grid, a four-dimensional hypercubic lattice in Euclidean space. Gauge field variables are placed on links following Eq. (1.3) in the obvious fashion,

$$U_\mu(n) = \exp\left[iagA_\mu^\alpha(n)\lambda^\alpha/2\right] \tag{1.5}$$

where μ labels the link direction, n is a quartet of integers labeling a site, a is the lattice spacing, and g is the gauge coupling at length scale a. The pure gluon action is then constructed from the simplest discrete versions of $W(c)$, Eq. (1.4), the product of four $U_\mu(n)$'s around a closed path of four links,

$$S = -(1/g^2)\sum(\operatorname{tr} UUUU + \text{h.c.}) \tag{1.6}$$

in an abbreviated but hopefully clear notation where the sum extends over all such paths, plaquettes, of the lattice. Equation (1.6) formulates $SU(3)$ gauge field dynamics in a fashion that ordinary statistical mechanics methods can cope with.

What are the major properties of the lattice formulation Eq. (1.6)? One can easily check that in a classical continuum limit ($a \to 0$, g fixed with smooth fields),

$$S \to \frac{1}{4}\int (F_{\mu\nu}^\alpha)^2 d^4x + O(a^2) \tag{1.7a}$$

where

$$F_{\mu\nu}^\alpha = \partial_\mu A_\nu^\alpha - \partial_\nu A_\mu^\alpha - g f_{\alpha\beta\gamma} A_\mu^\alpha A_\nu^\beta \tag{1.7b}$$

is the familiar gauge covariant field strength and $f_{\alpha\beta\gamma}$ are the structure constants of $SU(3)$. This classical analysis can be improved through the addition of weak coupling quantum fluctuations. Then the quantized conventional continuum gauge field formulation is found with a lattice coupling constant g^2 which must depend on a itself and which goes to zero as $a \to 0$. This is asymptotic freedom—the field fluctuations on length scales near the ultraviolet cutoff a become free as $a \to 0$. The approach to freedom is logarithmic,

$$g^2(a) = \frac{g_0^2}{1 + (cg_0^2/2\pi)\ln(a_0/a)}, \qquad c = 11/4\pi \tag{1.8}$$

This is a central result needed to understand the continuum limit of the lattice theory. It means that $g^2 = 0$ is an infrared unstable fixed point of the theory whose scaling laws can be obtained perturbatively. The resulting analytic control over the theory's continuum limit plays an important role in the estimates of quantitative properties of QCD, as will be illustrated in greater detail below.

Another important property of Eq. (1.6) is its computable strong coupling behavior. High-"temperature" expansions, i.e., in powers of $1/g^2$, show that when a static quark and antiquark are separated a distance R in the pure gluon theory, a flux tube forms between them and gives rise to a linear confining potential, $V(R) = \sigma R$. The coefficient σ is the "string tension" of considerable fame in heavy quark phenomenology and relativistic string models of high-energy scattering. Its experimental value is $\sqrt{\sigma} \approx 420$ MeV.

1.2. The Statistical Mechanics–Field Theoretic Dictionary

It is clear from Eq. (1.6) that the lattice gauge theory formulation of pure glue casts the theory into the form of a four-dimensional statistical mechanics. The path integral of the lattice theory is

$$Z = \int \left[\prod_{\mu,n} dU_\mu(n) \right] e^{-S} \tag{1.9}$$

and can be interpreted as a partition sum. The following correspondence between the two languages, some of which are obvious, follow:

Statistical mechanics	Field theory
Energy	Action
Temperature	Coupling
Free energy density	Vacuum energy density
Correlation function	Propagator
Correlation length	Reciprocal of the mass gap

These correspondences will give us a useful perspective into the lattice theory and its continuum limit, relativistic QCD.

1.3. Phases and Order Parameters of Lattice Gauge Theory

Consider the question of confinement in the pure gluon theory. We want to calculate the heavy quark potential $V(R)$ in a statistical mechanics setting. We need a gauge-invariant matrix element to describe this physical situation. Consider a closed world line of a quark shown in Fig. 1 and described as an external current J_μ^α. The closed path describes a simple thought experiment—separate a quark–antiquark pair adiabatically a distance R, hold that configuration for a long time $T \gg R$, then finally bring the pair back together again. The transition amplitude for this process in Euclidean space can be written as a path integral,

$$\langle i | e^{-HT} | f \rangle = \int [DA_\mu] \exp\left(-S + ig \int A_\mu^\alpha J_\mu^\alpha \, d^4x \right) \Big/ \int [Da_\mu] e^{-S} \tag{1.10}$$

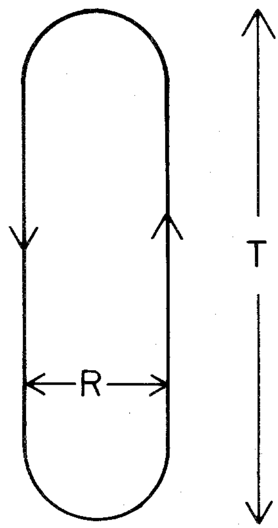

Fig. 1. A closed quark world line.

using continuum field theory notation for convenience. Here $|i\rangle$ and $|f\rangle$ are the "initial" and "final" configurations of the quarks—a pair separated a distance R—and H is the Hamiltonian of the pure gluon field theory. Over the time interval T, the quarks are static so H is pure potential. Call it $V(R)$. For pointlike quarks the right-hand side of Eq. (1.10) can also be simplified,

$$e^{-V(R)T} = \left\langle \operatorname{tr} P \exp\left(ig \oint_c A_\mu^\alpha \lambda^\alpha \, dx_\mu / 2 \right) \right\rangle \tag{1.11}$$

Or,

$$V(R) = -\lim_{T\to\infty} \frac{1}{T} \ln\langle W(c)\rangle \tag{1.12}$$

using the notation of Eq. (1.4) and identifying the closed contour C with Fig. 1.

Equation (1.12) allows us to identify $\langle W(C)\rangle$ as the "order parameter" for confinement.[4] There are two natural alternative behaviors for the dependence of $\langle W(C)\rangle$ on the geometry of the contour C.[5] First, $\langle W(C)\rangle$ may fall to zero as the exponential of the minimal area enclosed by C,

$$\langle W(C)\rangle \sim e^{-\sigma RT} \tag{1.13a}$$

which corresponds, using Eq. (1.12), to a confining heavy quark potential,

$$V(R) = \sigma R \tag{1.13b}$$

Another possibility is that $\langle W(C)\rangle$ falls off much more slowly, as the perimeter of C, say. Then, for $T \gg R$,

$$\langle W(C)\rangle \sim e^{-mT} \tag{1.14a}$$

and

$$V(R) = m \tag{1.14b}$$

characteristic of quarks which propagate freely at large distances.

The result Eq. (1.14b) is familiar to all, but linear confinement Eq. (1.13b) is not. By considering the high-temperature, i.e. strong coupling, expansion of $\langle W(C)\rangle$ we see that the strongly disordered character of the link variables causes confinement. Begin with

$$\langle W(C)\rangle = \int \Big[\prod_{\mu,n} dU_\mu(x) \Big] \prod_C U \times \exp\Big[-\frac{1}{g^2} \sum (\operatorname{tr} UUUU + \text{h.c.}) \Big] \Big/ \int [dU] e^{-S} \tag{1.15}$$

for rectangular contour of sides R and T, $T \gg R$, on the lattice. Since $\int [dU_\mu(n)] U_\mu(n) = 0$ and $\int [dU_\mu(n)] U_\mu^{\dagger\alpha\beta}(n) U_\mu^{\gamma\delta}(n) = \frac{1}{3} \delta_{\alpha\delta} \delta_{\beta\gamma}$, the first non-trivial term is found in the numerator of Eq. (1.15) in a $1/g^2$ expansion when the exponential contributes a factor of $-1/g^2 \operatorname{tr} UUUU$ for each plaquette inside C. This is shown in Fig. 2 and produces

$$\langle W(C)\rangle \sim (1/g^2)^{RT} = \exp(-\ln g^2 \cdot RT) \tag{1.16a}$$

So,

$$V(R) = \sigma R \tag{1.16b}$$

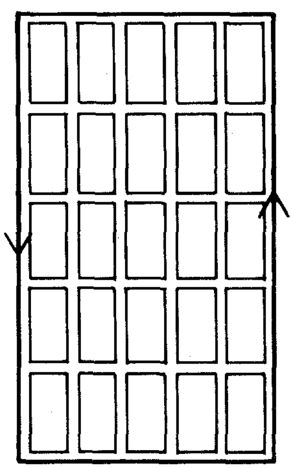

Fig. 2. Strong coupling expansion of the Wilson loop correlation function.

with

$$\sigma = \ln g^2 + \cdots \tag{1.16c}$$

in units of the lattice spacing a. Higher-order corrections to Eq. (1.16c) can be obtained in a systematic fashion.

The flux-tube picture of confinement follows from taking a fixed time slice of Fig. 2 and noting that the energy density and flux causing confinement occur in a thin tube between the quarks. Intriguing connections with strong models of hadronic structure can also be drawn.

It should be clear from these exercises that lattice gauge theory has much in common with the theory of two-dimensional fluctuating surfaces embedded in four dimensions. Recent research into the lattice theory and its mechanism of confinement has faced the issue of roughening of the flux-tube,[6] restoration of rotational symmetry in lattice calculations of heavy quark potential[7] and the character of the intrinsic width of the fluctuating surface. An intriguing result of this approach was the discovery of a universal $1/R$ term in the heavy quark potential,[8]

$$V(R) = \sigma R - \frac{\pi/12}{R} + \cdots \tag{1.17}$$

which should be characteristic of any four-dimensional flux tube model of confinement in a relativistic theory.

Now we turn to another order parameter of strong interactions—dynamical mass generation of quarks. Since chiral symmetry and massless quarks may not be familiar to many statistical mechanics theorists, let me begin this discussion with a brief review of conventional QCD thoughts on the subject. Consider the theory with a doublet of massless quarks, $\psi = \binom{u}{d}$, where each quark comes in three colors, u_i, d_i with $i = 1$, 2, and 3. The QCD action is,

$$S = -\frac{1}{4}\int (F^{\alpha}_{\mu\nu})^2 d^4x + \int \bar{\psi}(i\not{\partial} + g\not{A}^{\alpha}\lambda^{\alpha})\psi\, d^4x \tag{1.18}$$

The absence of bare masses for the quarks implies that the left- (L) and right-handed (R) quark fields do not couple together in S and the theory is symmetric under $SU(2)_L \otimes SU(2)_R$ continuous transformations. The axial $SU(2)$ is particularly interesting,

$$\binom{u}{d}' = e^{i\gamma_5 \mathbf{T}\cdot\mathbf{n}\theta}\binom{u}{d}, \qquad 0 < \theta < 2\pi \tag{1.19}$$

where T_i is a generator of the $SU(2)$ "flavor" symmetry. This is an exact global symmetry of the action for massless quarks. Phenomenology indicates, however, that this symmetry is spontaneously broken by the theory's vacuum. In this way a triplet of massless bosons, the pions π^+, π^0, and π^-, appear in the spectrum as the Nambu–Goldstone bosons of the spontaneously broken continuous symmetry. In the real world the small but finite pion masses ($m_\pi \approx 135$ MeV) are thought to reflect some explicit chiral symmetry breaking in the action itself (quark masses of several 5–7 MeV are favored phenomenologically—these are tiny masses on the scale of typical hadron masses of 1 GeV). In addition, the spontaneous breaking of the axial symmetry leads to successful low-energy scattering theorems, the analog of spin wave scattering results in the context of ferromagnets. In addition, there is an order parameter $\langle\bar{\psi}\psi\rangle \neq 0$ and the appearance of a dynamically generated mass for the quarks themselves. These results are all favored by phenomenology and generic current algebra analyses of QCD.

Later in this paper, after lattice fermions have been discussed, we shall return to the numerical evidence for the breakdown of chiral symmetry in the theory's continuum limit. In the continuum theory the appearance of a nonzero $\langle\bar{\psi}\psi\rangle$ is a nonperturbative effect—$\langle\bar{\psi}\psi\rangle$ vanishes order by order in weak coupling expansions using Eq. (1.18) because of the algebraic symmetry Eq. (1.19)—which indicates that the quark–antiquark attraction is sufficient to cause condensation of pairs. There is an amusing, instructive, but very intuitive and informal connection between s-wave bound state formation in theories of confinement and chiral symmetry breaking.[9] Suppose that an s-wave bound state occurs in a theory due to a spin-independent, attractive force between quark–antiquark pairs. The confining force of lattice gauge theory is such a phenomenon. Suppose also that a simple two-body semiclassical approximation describes the s-wave bound state. Then, one can argue that quark–antiquark condensation must have occurred in the theory and $\langle\bar{\psi}\psi\rangle \neq 0$. To see this consider the bound state as depicted in Fig. 3. At a turning point in the quark's semiclassical

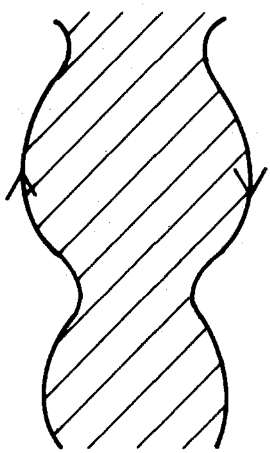

Fig. 3. A quark–antiquark bound state propagating in time.

trajectory, its momentum flips $\mathbf{p} \to -\mathbf{p}$, but its spin does not, $\mathbf{s} \to \mathbf{s}$. Therefore, its chirality $\mathbf{p} \cdot \mathbf{s}$ changes sign and we learn that its chirality is *not* a good quantum number and the symmetry of interest must be spontaneously broken. This little argument suggests that confining forces cause chiral symmetry breaking. This result has some support from computer simulations, as will be discussed later.

2. RECENT DEVELOPMENTS IN GLUON THEORIES

Our theoretical and numerical grasp of the pure gluon sector Eq. (1.6) is much firmer than our understanding of QCD with dynamical, light fermions. Therefore, let us review that aspect of QCD first and later discuss the problems with fermions.

The pure gluon theory confines static quarks at strong coupling as discussed above. In fact, it has been proved that the lattice theory confines for all g^2 different from zero.[10] The proof relies on the non-Abelian character of the gauge group [the proof has been developed only for $SU(2)$] and uses Migdal–Kadanoff renormalization group transformations to establish bounds on $\langle W(C) \rangle$. These results in turn show that the string tension is nonzero for all g^2.

This result leaves us, however, with the hard problem of determining whether confinement is a property of the continuum limit of the lattice theory and whether the continuum limit yields a sensible, relativistic field theory. On these topics we have only numerical evidence, but the tentative answers are "yes" in both cases. Recall that asymptotic freedom governs the approach to the continuum limit. It defines the scaling laws of physical quantities for couplings g^2 in the vicinity of the unstable free-field fixed point $g^2 = 0$. The scaling lows are obtained by a familiar argument. Suppose M is a physical mass of the theory. When calculated using lattice techniques it depends on both a and g^2. However, it is renormalization group invariant,

$$\frac{d}{da} M(g^2, a) = 0 \tag{2.1}$$

In addition, by dimensional analysis,

$$M(g^2, a) = \frac{1}{a} f(g^2) \tag{2.2}$$

These equations imply that

$$f'(g) = -f(g)/\beta(g) \tag{2.3a}$$

where

$$\beta(g) = -a \frac{dg}{da} \tag{2.3b}$$

is the Callan–Symanzik function. These equations mean that when one computes a physical quantity such as M on lattices of different spacings, the coupling g will have to be adjusted accordingly. But $\beta(g)$ can be computed in perturbation theory,

$$\beta(g) = -\beta_0 g^3 - \beta_1 g^5 - + \cdots \tag{2.4a}$$

where

$$\beta_0 = \frac{11}{3}\left(\frac{N}{16\pi^2}\right), \qquad \beta_1 = \frac{34}{3}\left(\frac{N}{16\pi^2}\right)^2 \tag{2.4b}$$

for $SU(N)$ gauge theories.[11] The famous minus signs in Eq. (2.4) indicate asymptotic freedom—as $a \to 0$, $g^2 \to 0$ also. Using Eq. (2.3a) the scaling law for $M(g^2, a)$ becomes

$$M^i = C^i \cdot \frac{1}{a}\left(\beta_0 g^2\right)^{-\beta_1/2\beta_0^2} e^{-1/2\beta_0 g^2}\left[1 + O(g^2)\right] \tag{2.5}$$

where i labels various masses of the theory and the C^i are pure numbers. There are several important features of this result. First, the appearance of a mass in the theory is a nonperturbative effect—M^i depends on g^2 with an essential singularity at $g^2 = 0$. Second, mass ratios are pure numbers which are independent of g^2. They are universal and depend only on the gauge group. The theory is very predictive! And third, the verification of the scaling law Eq. (2.5) is an essential ingredient in any good calculation of the continuum properties of the lattice theory.

This last point consumes much of the attention of theorists who calculate the string tension of the $SU(3)$ using computer simulation methods. A rough sketch of the data from an $8 \times 8 \times 8 \times 8$ lattice is shown in Fig. 4. There is a narrow window in coupling $g^2 \approx 1$ where small lattices appear to yield good estimates of physical quantities and their scaling laws. However, on such small lattices, systematic effects are always present (finite size problems), and the uncertainty in the overall mass scale of the theory is considerable. Workers in the field believe that systematic uncertainties of $\pm 100\%$ affect the present generation of computer simulations.

Many other physical quantities have been estimated by these techniques. Pure gluonic energy levels ("glueballs") and quark model calculations of meson and baryon masses have been made. All of these results are encouraging and interesting. However, researchers are now trying to determine the reliability of their calculations, and are trying to put meaningful error estimates on their results. There are two problems here. First, the lattice itself—the fine grid work—is a distortion of space-time so corrections of $O(a)$ exist. And second, the volume V of the lattice box is finite so corrections of $O(V^{-1})$ must be expected. Both of these problems can be

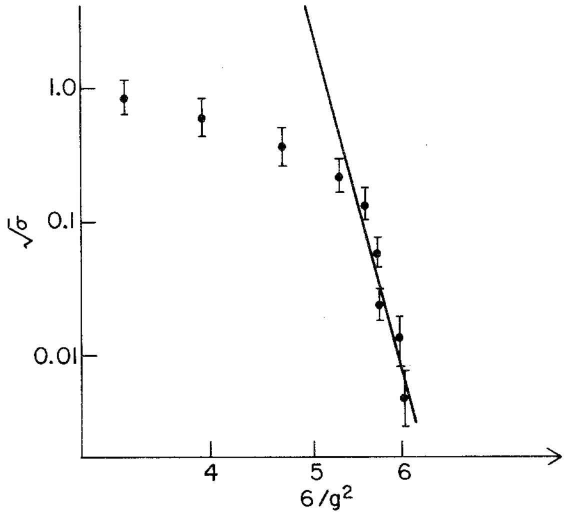

Fig. 4. Monte Carlo data for the string tension. The straight line on the log plot represents the asymptotic freedom scaling law.

dealt with systematically—the $O(a)$ corrections can be reduced by improving the lattice action and the $O(V^{-1})$ can be isolated by doing finite-size scaling studies. Let us discuss the $O(a)$ corrections. Recall that classical analysis gave

$$S \to \frac{1}{4} \int (F^{\alpha}_{\mu\nu})^2 d^4x + O(a^2) \tag{2.6}$$

as the lattice spacing $a \to 0$. A better fit to the continuum action can be made by adding irrelevant operators to S to reduce the $O(a^2)$ error to $O(a^4)$. Consider a trivial free-field example before discussing the gauge theory. A free scalar field has the action

$$S_0 = -\frac{1}{2} \sum_m \phi(n) \nabla^2 \phi(n) \tag{2.7a}$$

where ϕ is defined on sites n and a discrete form of the second derivative is

$$\nabla^2 \phi(n) = \sum_\mu \left[\phi(n+\mu) + \phi(n-\mu) - 2\phi(n) \right] \tag{2.7b}$$

It is easy to now calculate the inverse propagator for the scalar excitation,

$$\frac{4}{a^2} \sum_\mu \sin^2(p_\mu a/2) = p^2 - \frac{1}{12} a^2 \sum_\mu p_\mu^4 + \cdots \tag{2.8}$$

and obtain the $O(a^2)$ corrections to the continuum result. But if we add a term $O(a^2)$ to S, an irrelevant ∇^4 coupling,

$$S_0 \to S_0 - \frac{1}{24} a^2 \sum_n \phi(n) \nabla^4 \phi(n) \tag{2.9a}$$

the inverse propagator becomes

$$\frac{4}{a^2} \sum_\mu \left[\sin^2(p_\mu a/2) + \frac{1}{3} \sin^4(p_\mu a/2) \right] = p^2 - \frac{1}{90} a^4 \sum_\mu p_\mu^6 + \cdots \tag{2.9b}$$

and a better fit to p^2 is obtained.

In lattice gauge theory one can add to the "four-spin" interaction term "six-spin" terms with appropriate weights so that

$$S_{\text{improved}} = \frac{1}{g^2} \left(\sum c_4 \text{tr}\, UUUU + \sum c_{6,i} \text{tr}\, UUUUUU \right)$$

$$\to \frac{1}{4} \int (F_{\mu\nu}^\alpha)^2 d^4x + O(a^4) \tag{2.10}$$

So, in addition to closed paths of length $a \times a \times a \times a$, closed paths of six links appear in the lattice action and choosing the coefficients c_4 and $c_{6,i}$ (i labels the different types of 6-link closed paths) correctly the error is reduced to $O(a^4)$. This improvement program can also be carried out on the propagators of interest—correlation functions of two tr $UUUU$ operators—to improve mass spectrum calculations.

We have illustrated these ideas in classical analysis and free-field cases. They also can be applied systematically to interacting theories. For asymptotically free theories one can calculate the improvement coefficients c_4, $c_{6,i}$, etc. order by order in perturbation theory.[12] The estimates given above are then altered by logarithms of a, $O(a^2) \to O(a^2 \ln a)$, for example. The logarithms occur because of asymptotic freedom, $g^2 \sim 1/\ln(1/a)$.

This perturbative and systematic program for improving the lattice actions of asymptotically free theory has been set down for four-dimensional gauge theories, but has not been applied extensively. An impressive model calculation, the $O(3)$ Heisenberg magnet in two dimensions, was carried out through one-loop order and the theory's dynamically generated correlation length was computed by simulating the improved action.[13] Asymptotic freedom was found for the correlation length ξ in analogy to Fig. 4. In fact, the improved action gave the continuum scaling law even when ξ and a were comparable! This then permitted improved studies of ξ as a function of g^2, the verification of dynamical mass generation, scaling, and the determination of the scale of ξ itself. It was found that previous more naive calculations of ξ underestimated it by factors of 3–4! The lesson learned was that although naive calculations gave good evidence for scaling, the scales of physical quantities were affected by irrelevant operators whose effects vanish slowly as $a \to 0$ and these effects shifted the curve of ξ vs. $1/g^2$ leading to a poor determination of ξ itself. Some of the earlier calculations were quite nontrivial. They include simulations on 100×100 lattices,[14] a Monte Carlo renormalization group calculation,[15] and Hamiltonian strong coupling expansions.[16] The straightforward Monte Carlo simulations using the simplest nearest-neighbor coupled action,

$$S = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad \mathbf{S}_i^2 = 1 \tag{2.11}$$

found a scaling region for $\xi \gtrsim 5a$. Finite size effects are large when $\xi \approx 20a$ on a 100×100 lattice, so the scaling window covered the region $\xi = (5\text{–}20)a$. With the improved action a much more impressive fit to asymptotic freedom was achieved because $\xi \approx a$ data were not affected significantly by the lattice grid.

This result casts doubts on the reliability of the string tension measurements in $SU(3)$ gauge theory. A good study with an improved action looks essential. Simply running simulations of the naive action on larger lattices may not expose the dangerous irrelevant operators which could be masking the scales. There is, in fact, evidence for such irrelevant operators in present computer simulations[17]—recent simulations on larger lattices produce smaller values for $\sqrt{\sigma}$—and in old Hamiltonian strong coupling expansions.[18]

This perturbative correction program removes a class of nonscaling effects in the vicinity of $g^2 = 0$. There may be other important nonperturbative effects complicating the theory at finite g^2. In $SU(3)$ gauge theory there certainly are such problems—the crossover near $g^2 \approx 1$ from strong coupling behavior to asymptotic freedom is very abrupt in the theory with the naive action and the theory's specific heat has a large, sharp peak in the vicinity of $g^2 \approx 1$. The "cause" of this effect was explained through a study of a generalized naive model, a "mixed" model,[19]

$$S = \frac{1}{g_F^2} \sum \mathrm{tr}_F\, UUUU + \frac{1}{g_A^2} \sum \mathrm{tr}_A\, UUUU + \text{h.c.} \tag{2.12}$$

where tr_F (tr_A) indicates a trace in the fundamental (adjoint) representation of the gauge group. For small fluctuations of the link variables U around the identity, the representation of the group does not affect the physics. However, in the intermediate and strong coupling regions $g^2 \gtrsim 1$, the global character of the group representation is important and the mixed model has some special features. Computer simulations revealed the phase diagram in the (g_A, g_F) plane shown in Fig. 5. The dotted lines indicate first-order transitions. Note that the line of first-order transitions terminates (at a critical point, presumably) near the "pure fundamental action" line and

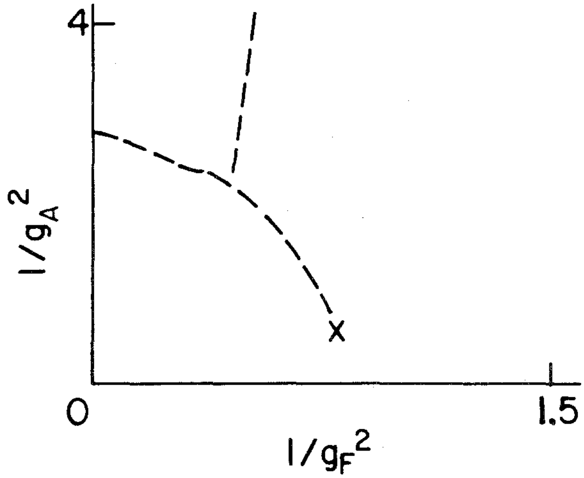

Fig. 5. Phase diagram for the "mixed" model.

near $g_F^2 \approx 1.0$. So, the pure naive action model "almost" has a phase transition. This certainly affects the lattice theory's approach to the continuum limit. To evade the problem one should continue to work with the mixed model but choose a path to the continuum fixed point $(g_F^2, g_A^2) = 0$ which evades the nearby critical point, i.e., add some $\mathrm{tr}_A\, UUUU$ with a negative weight to the naive action. The resulting mixed model could also be perturbatively improved in the vicinity of the fixed point. To my knowledge, such a thorough study has not been done yet.

3. LATTICE FERMIONS: CONCEPTUAL ISSUES AND NUMERICAL METHODS

Now we wish to put massless quarks into the model and discuss chiral symmetry and hadron mass spectroscopy. To begin we must consider a discrete form of the Dirac equation. The reader will quickly discover, if he tries this exercise, that it is deceptively tricky. In fact there are some precise NO-GO theorems on this subject.[20] For example, you cannot

1. describe a single left-handed quark with a "conventional" action on the lattice;
2. nor can you describe a multiplet of quarks with all the continuous axial flavor symmetries with a "conventional" lattice action.

The term "conventional" here includes the properties of locality and hermiticity and is essential in these results.[20]

We can understand the origins of these limitations by considering several simple examples.[21] Consider a one-dimensional spatial lattice in a temporal continuum. Place a two-component Dirac field $\psi(n)$ on each site n. The most naive discrete form of the Dirac equation would then be

$$i\dot{\psi}(n) = -\frac{i}{2a}\gamma_5[\psi(n+1)-\psi(n-1)] \tag{3.1a}$$

to approximate the continuum Dirac equation,

$$i\dot{\psi}(n) = -i\gamma_5\partial_z\psi(n), \qquad \gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{3.1b}$$

To obtain the low-energy content of Eq. (3.10) we consider plane waves,

$$\psi_\pm = e^{i(-kna+Et)}\chi_\pm \tag{3.2a}$$

and chiral eigenstates,

$$\gamma_5\chi_\pm = \pm\chi_\pm \tag{3.2b}$$

Substituting into Eq. (3.1a) gives the energy-momentum relation,

$$E = \pm\sin(ka)/a$$

which is plotted in Fig. 6. So, the lattice regulator has produced low energy excitations at $ka \approx 0$ as well as $ka \approx \pm\pi$. The continuum limit of Eq. (3.1a) has two fermion species, each fermion accompanied by a partner with canceling chirality. This is the infamous problem of "species doubling."

Let us consider two attempts to make a more suitable lattice Dirac equation. In the first, an illustration of a proposal by Wilson, we add an

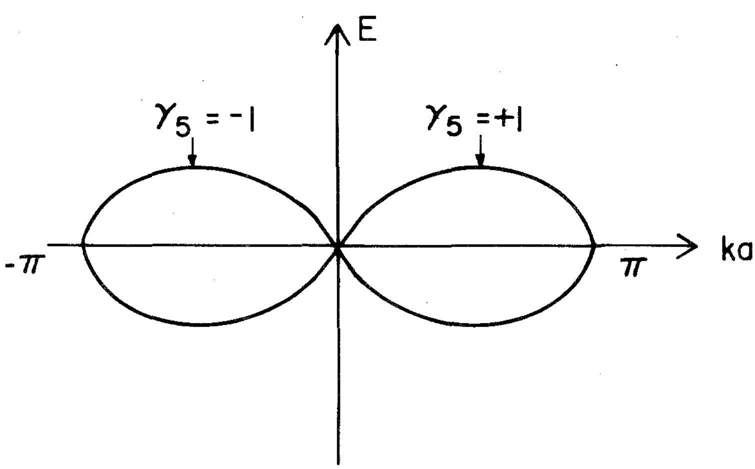

Fig. 6. Dispersion relation for free fermions on a discrete space–continuum time lattice.

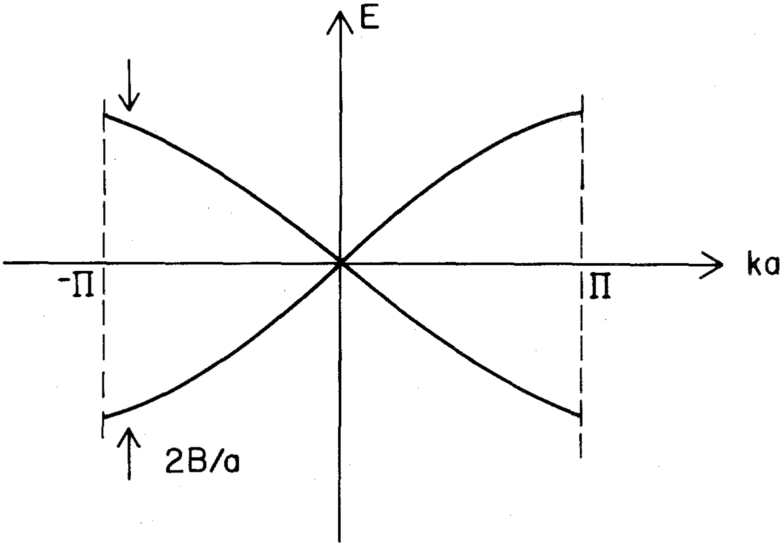

Fig. 7. Dispersion relation for free Wilson fermions.

irrelevant term to the naive Hamiltonian[21] to raise the energy of the $E - k$ relation near $ka = \pm\pi$,

$$H = -\frac{i}{2a}\sum_n \psi^\dagger \gamma_5 \partial_z \psi + \frac{B}{2a}\sum_n \bar{\psi}\nabla^2\psi \tag{3.3}$$

The resulting energy-momentum relation is shown in Fig. 7. Now one species emerges in the continuum limit. However, we have paid a dear price. The irrelevant term in Eq. (3.3) breaks chiral symmetry $\psi \to e^{i\gamma_5\theta}\psi$ completely. This means that when interactions are added to the model, there is no symmetry in the Hamiltonian to prevent mass counterterms. Therefore, another term must be added to H to cancel off the induced mass term in order to have massless fermions in the Hamiltonian itself. This adjustment precludes a satisfactory first principles study of chiral symmetry and its possible spontaneous breakdown due to interactions in QCD. It also makes it difficult to study the hadron spectrum in the physically relevant light quark sector.

A different approach to the problem thins the lattice degrees of freedom in order to produce but one species in the continuum limit. It places the upper component of $\psi(n)$, call it ψ_1, on odd sites of the lattice and the lower component, ψ_2, on even sites. The Hamiltonian is then[21]

$$H = -\frac{i}{2a}\sum \left[\psi_1^\dagger(n)\psi_2(n+1) - \psi_2^\dagger(n+1)\psi_1(n)\right] \tag{3.4}$$

One can then obtain the equations of motion for ψ_1 and ψ_2, reconstruct the Dirac equation, Eq. (3.16), and find one species in the continuum limit. What is the cost of this method? For $a \neq 0$ it only has discrete pieces of continous chiral symmetry ($\psi \to \gamma_5 \psi$, only) because upper and lower components of ψ are on different sites. This symmetry is sufficient, however, to forbid dynamically generated mass counterterms and it ensures the restoration of continuous chiral symmetry in the continuum limit. Therefore, the method is interesting for QCD although the strongly cutoff model has less symmetry than its continuum limit.

The reader might reconsider the generic limitations of lattice fermions discussed at the opening of this section and consult the literature for proofs of the NO-GO theorems. They build upon the features found in the explicit exercises done above.

Now let us discuss numerical methods for fermions. This is a difficult, unfamiliar subject for most statistical mechanics theorists because of the anticommuting property of Euclidean fermions. These variables are difficult to deal with numerically because of the apparent nonlocal character of their anticommutation rules. Consider the action of lattice QCD written in a generic fashion,

$$S = \sum_{ij} \bar{\psi}_i [\not{D}(U) + m]_{ij} \psi_j + S_0(U) \tag{3.5}$$

where $S_0(U)$ is the pure gluon action and the first term is the quark kinetic energy in a discrete form. The $\not{D}(U)$ is a discrete form of the covariant derivative. The details of this form of the action depend on the lattice fermion method one uses. Our analysis will be generic, so $\not{D}(U)$ will suffice for us. Of course, the quark hopping term must be locally gauge invariant. This is ensured by writing a string of U matrices between $\bar{\psi}$ and ψ so that color indices are all locally contracted into local color singlets [e.g., $\bar{\psi}(n)$ $U_\mu(n)\psi(n+\mu)$ is allowed].

How can we handle Eq. (3.35) numerically? The path integral reads

$$Z = \int \prod_{n,\mu} dU_\mu(n) \prod d\psi \prod d\bar{\psi}\, e^{-S} \tag{3.6}$$

and it does not have a simple statistical mechanics interpretation because the ψ's are anticommuting variables. However, since ψ and $\bar{\psi}$ enter S only quadratically we can integrate them out by standard methods,

$$Z = \int \prod_{n,\mu} dU\mu(n) \det{}^{N_f}[\not{D}(U) + m] e^{-S_0(U)} \tag{3.7}$$

where the infamous fermion determinant has appeared raised to the power N_f, the number of fermion species (flavors). Equation (3.7) can be written in the form

$$Z = \int \prod_{n,\mu} dU_\mu(n)\, e^{-S_{\rm eff}} \tag{3.8a}$$

with

$$S_{\rm eff} = S_0(U) - N_f \operatorname{tr} \ln\left[\not{D}(U) + m \right] \tag{3.8b}$$

Unfortunately, the tr ln term in Eq. (3.8b) gives long-range couplings in the effective action, so it is difficult to deal with analytically. However, there is a direct, brute-force way to simulate Eq. (3.8b) which might permit numerical studies of lattice QCD.[22] Suppose we study Eq. (3.8b) with a Monte Carlo method such as the Metropolis algorithm. Then we only need the differences of $S_{\rm eff}$ before and after a local change in the gauge field configuration. Since the matrix $[\not{D}(U) + m]$ is sparse (only nearest neighbors are coupled), the difference of actions can be calculated with a local, stochastic algorithm. To be specific, change one link variable in the configuration $\{U\}$. Call the new configuration $\{\tilde{U}\}$ and let the local change be small. Then the change in $S_{\rm eff}$ is

$$S_0(\tilde{U}) - S_0(U) - \sum_{ij} G_{ij}(U) \frac{\delta \not{D}(U)_{ij}}{\delta U} (\tilde{U} - U) + O\left[(\tilde{U} - U)^2 \right] \tag{3.9}$$

where G_{ij} is the fermion Green's function in the background gauge configuration $\{U\}$. This equation suggests an algorithm:

1. Consider a fixed $\{U\}$ and the boson action

$$S(\phi) = \sum_{ij} \phi_i^* \left[\not{D}(U) + m \right]_{ij} \phi_j \tag{3.10a}$$

Calculate $G_{ij}(U) = \langle \phi_i^* \phi_j \rangle$ for this model by ordinary Monte Carlo methods.

2. Update the gauge field with a small change $\{U\} \rightarrow \{\tilde{U}\}$ using the action

$$S(U) = S_0(U) - \sum_{ij} G_{ij} \left[\not{D}(U) + n \right]_{ij} \tag{3.10b}$$

3. Go to step 1 and repeat.

In the limit of small changes $\{U\} \rightarrow \{\tilde{U}\}$, this method simulates Eq. (3.8b) exactly. Preliminary studies of it are fairly encouraging—one to two orders of magnitude more computing power than used for ordinary gauge theory simulations appear necessary. The method, however, has not been applied to QCD with light quarks yet, so its promise is not really verified.

This is the pseudofermion method. It was introduced in Ref. 22, and the reader should consult the literature for more technically complete discussions.

One of the many potential problems with the pseudofermion stochastic method is the difficulty of doing error and convergence analysis for it. Most workers in the field believe that other methods are needed to solve the fermion simulation problem. A unique and very promising method based on the microcanonical ensemble is being developed and tested at this time.[23] In it classical equations of motion using ordinary boson variables in four Euclidean plus one time dimension are simulated. The ensemble averages of the canonical ensemble are replaced by time averages of the microcanonical ensemble. Some cleverness is needed in constructing the microcanonical action in order that it correspond to the canonical ensemble Eq. (3.8), and that has been done. The method's equations of motion are not hard to simulate numerically and work is underway on $SU(2)$ and $SU(3)$ gauge theories with four flavors of massless quarks in four dimensions. Since similations of equations of motion are subject to standard convergence criteria, the method is controlled and clear. Results of physical calculation are eagerly awaited.

4. APPLICATIONS, RESULTS, AND NEW DIRECTIONS

Let me first review very briefly the type of work which has been done recently. There have been encouraging computer simulations of the hadron spectrum in the $N_f \to 0$, or quenched approximation.[24] In this limit the infamous fermion determinant becomes an innocuous unity and calculations are very simple. High-energy phenomenology suggests that the $N_f \to 0$ limit in which internal virtual quark loops are ignored may be a good qualitative guide to the low-energy mass spectrum. The Feynman diagrams the approximation includes in the calculation of a meson propagator are shown in Fig. 8. The quarks literally move in the gluon field theory and the absence of internal quark loops means that the fermions themselves do not feed into the dynamics. The computer calculation of the quark propagators needed in such a calculation of a composite meson propagator is not difficult. How good are the results for the π, ρ, ω, ϵ, P, Δ, N, Ξ, etc? They all look encouraging, but are still under extensive study. Finite size effects, finite quark mass errors, etc. plague the present generation of calculations.

Chiral symmetry has also been studied, and using a four-dimensional Euclidean version of the scheme Eq. (3.4) good evidence for spontaneous symmetry breaking has been found.[25] The Goldstone–Nambu physical picture of the pion appears to result properly.

QCD in the quenched approximation has also been studied in extreme environments—high temperatures and in dense nuclear matter. Deconfinement in $SU(3)$ gauge theory and chiral symmetry restoration at $T_c \approx 200$ MeV has been discovered and the transitions are strongly first order.[26] Large latent heats have been discovered and they may be relevant to the early life of the universe and they may be explored in heavy-ion

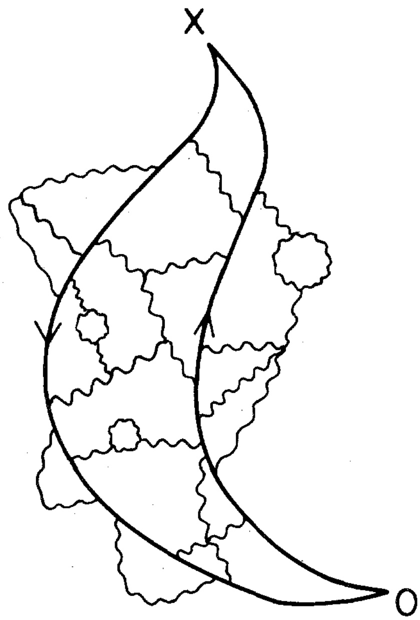

Fig. 8. Feynman diagrams contributing to the quenched calculation of a meson propagator.

collisions. Chiral symmetry restoration in dense nuclear matter has also been seen,[27] but quantitative studies are lacking. The physics of extreme environments is a particularly attractive scene for lattice gauge theory. The quenched approximation is quite questionable here and much work is being expended to improve these calculations.

Finally a few words about future directions. It would be interesting to study symmetry breaking in grand unified theories. Realistic models are probably beyond our reach because of the NO-GO theorems on lattice fermion methods. Nonperturbative effects in supersymmetric models represent new ground which lattice gauge theory might attack. Lattice supersymmetry in various forms is being studied by several groups. On the analytic front, special methods exist for $N \to \infty$ theories (N = number of colors) and elegant connections with string models appear possible.

Lattice gauge theory should continue as a useful method for studying field theories for the next few years.

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