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Monte Carlo simulation II: measuring observables

Regarding the lattice as merely an ultraviolet cutoff, we would like to use the Monte Carlo simulation technique for the calculation of some physical numbers characteristic of the continuum field theory. At the outset it is not clear how well this can be done with the rather limited lattices available. For believable results we must make the lattice spacing smaller than relevant hadronic scales and yet have the overall lattice larger than the scale of physics we are measuring. A lattice of order 10 sites in any given direction leaves little leeway in such an analysis. Furthermore, the renormalization group discussion of chapter 13 points out that we should expect an exponential dependence of the lattice spacing on coupling constant. At best only a very narrow range of coupling can be useful in extracting physical numbers.

To counteract this pessimism, we have the remarkable experimental fact that the scaling behavior predicted by asymptotic freedom appears in deep inelastic scattering experiments at the precociously low momentum transfers of order 2 GeV (Perkins, 1977). Thus our 10^4 site lattices may give interesting results for physics at energy scales down to a few hundred MeV, exactly where strong confinement forces should come into play. Thus we may hope to relate a few features of long- and short-distance quark dynamics.

We should attempt to measure a quantity which has a finite continuum limit; that is, we must extract a physical observable. The average plaquette, which dominated the above Monte Carlo discussion, is proportional to the expectation value of the action density and is expected at the perturbative level to have ultraviolet divergences. The simplest physical observable for extraction from a Monte Carlo analysis is K, the coefficient of the linear long-range interquark potential. This may be found by measuring large Wilson loops and looking for the area law falloff discussed in chapter 9. Measuring distances in lattice units, one actually determines the dimensionless combination a^2K as a function of the bare coupling g_0^2. If the linear potential survives the continuum limit, the weak coupling behavior of this combination should follow the prediction of the renormalization group as

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discussed in chapter 13.

$$a^2K = (K/\Lambda_0^2)\,(\gamma_0 g_0^2)^{(-\gamma_1/\gamma_0^2)} \exp\left(-1/(\gamma_0 g_0^2)\right)(1+O(g_0^2)). \tag{19.1}$$

Conversely, verification of this behavior will provide strong evidence for the survival of the linear potential when the cutoff is removed.

In general the behavior of a Wilson loop can be quite complicated. In addition to the area law piece dominant for large loops, there should be perimeter dependence from the self energies of the quark sources and yet further corrections from perturbative gluon exchange across the loop. As the coupling is reduced and the continuum limit approached, the perimeter piece should diverge and dominate for any fixed size loop. To eliminate this distraction, it is convenient to consider ratios of loops with different areas but the same perimeter. In particular, define (Creutz, 1980*c*)

$$\chi(I,J) = -\ln\left(\frac{W(I,J)\,W(I-1,J-1)}{W(I,J-1)\,W(I-1,J)}\right), \tag{19.2}$$

where $W(I,J)$ denotes the expectation of a rectangular Wilson loop of lattice dimensions I by J. In these quantities any perimeter dependence or constant factors in the loops will cancel. Whenever the loops are dominated by an area law, $\chi(I,J)$ directly measures the string tension

$$\chi \to a^2K. \tag{19.3}$$

This occurs either when I and I are large or when the bare coupling is large. However, in the weak coupling limit gluon exchange should dominate and χ will have a perturbative expansion

$$\chi(I,J) = O(g_0^2). \tag{19.4}$$

For example the weak coupling expression for the one-by-one loop implies

$$\chi(1,1) = \begin{cases} 3g_0^2/16 + O(g_0^4), & SU(2) \\ g_0^2/3 + O(g_0^4), & SU(3). \end{cases} \tag{19.5}$$

Such a power behavior is in marked contrast to the essential singularity on the right hand side of eq. (19.26). To summarize, for strong coupling we expect all $\chi(I,J)$ to become the area law coefficient but as g_0^2 is reduced, smaller loops should give a χ deviating from the true a^2K. Thus the curves of $\chi(I,J)$ for all I and J should form an envelope along the curve of the string tension. For weak coupling this envelope should satisfy eq. (19.1).

In figure 19.1 we plot $\chi(I,I)$, for I up to four, as a function of g_0^{-2} for the gauge group $SU(2)$. At strong coupling the large loops have large relative errors but are consistent with χ approaching the values from smaller loops. The graph also indicates the strong coupling limit for the string tension

$$a^2K = \ln(g_0^2) + O(g_0^{-4}). \tag{19.6}$$

The weak coupling behavior of eq. (19.1) is shown as a band representing values of the parameter Λ_0 in the range

$$\Lambda_0 = (1.3 \pm 0.2) \times 10^{-2} K^{\frac{1}{2}}, \quad SU(2). \tag{19.7}$$

This error is a purely subjective estimate.

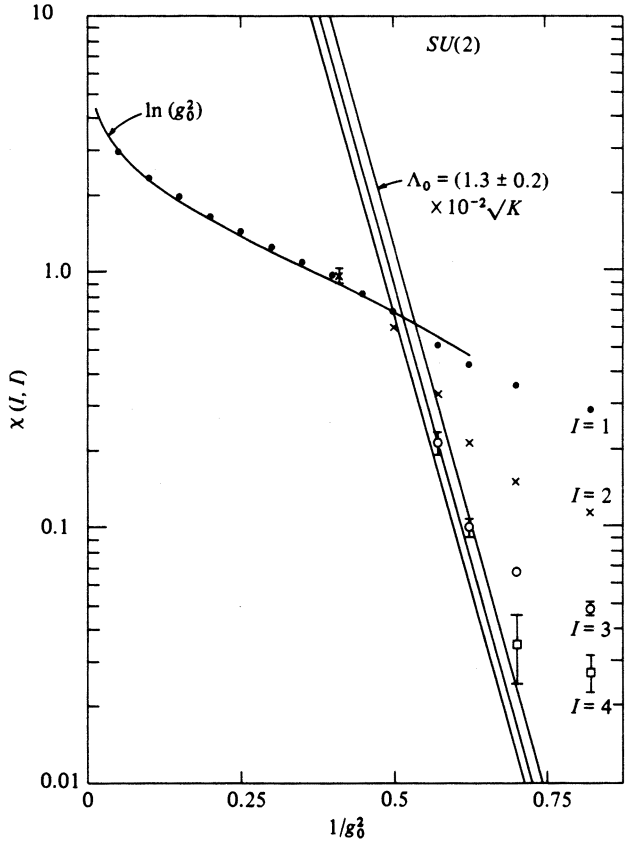

Fig. 19.1. Extracting the string tension for $SU(2)$ (Creutz, 1980*c*).

Figure 19.2 shows the same quantities for the gauge group $SU(3)$ on a 6^4 site lattice (Creutz and Moriarty, 1982*b*). On this smaller lattice, only loops up to 3-by-3 were used. For this theory the strong coupling expansion gives

$$a^2K = \ln(3g_0^2) + O(g_0^{-2}). \tag{19.8}$$

Note that the corrections for $SU(3)$ begin in a lower order of the strong coupling expansion than for the $SU(2)$ case in eq. (19.6). The weak coupling band for Λ_0 is now

$$\Lambda_0 = (6.0 \pm 1.0) \times 10^{-3} K^{\frac{1}{2}}, \quad SU(3). \tag{19.9}$$

When first obtained, these small numbers were quite surprising, coming as they do from theories with no small dimensionless parameters. However, as discussed in chapter 13, the value of Λ_0 is strongly dependent on renormalization scheme. There we quoted the results of Hasenfratz and

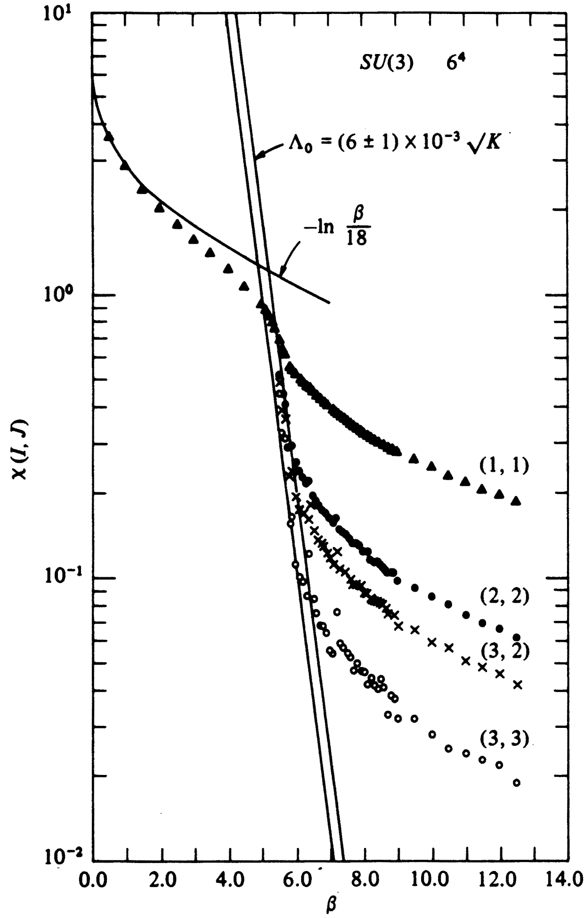

Fig. 19.2. Extracting the string tension for $SU(3)$ (Creutz and Moriarty, 1982*b*).

Hasenfratz, relating the lattice Λ_0 to the more conventional scale Λ_R defined by the three-point vertex in Feynman gauge and at a given scale in momentum space

$$\Lambda_R = \begin{Bmatrix} 57.5\Lambda_0, & SU(2) \\ 83.5\Lambda_0, & SU(3). \end{Bmatrix} \tag{19.10}$$

These large factors compensate the small numbers for Λ_0.

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To compare these results with real experiments, we need some idea as to the expected value for K. This is provided by the string model (Goddard *et al.*, 1973), wherein a rotating string gives rise to a Regge trajectory of particle states. The slope of this trajectory in terms of the string tension is

$$\alpha' = (2\pi K)^{-1}. \tag{19.11}$$

Using the phenomenological $\alpha' = 1.0\ \text{GeV}^{-2}$, we find

$$K^{\frac{1}{2}} = 400\,\text{MeV} = (14\ \text{tons})^{\frac{1}{2}}. \tag{19.12}$$

Combining this with eq. (19.9) and (19.10), we conclude

$$\Lambda_R = 200 \pm 35\,\text{MeV}. \tag{19.13}$$

The current phenomenological value for this parameter is rather uncertain but consistent with this value. Such a direct comparison should be regarded with some caution, however, because the above calculation does not take account of virtual quark effects.

Despite its uncertainties, the above analysis is a rather remarkable, first principles calculation of a physical parameter relating opposite distance extremes. The scale Λ relates to short-distance scaling phenomena and K represents long-distance confinement effects. Their ratio is a number totally inaccessible to perturbative treatments. It characterizes the solution of a hopefully non-trivial four-dimensional field theory.

A second number of interest for Monte Carlo analysis is the mass gap or correlation length of the theory. This was discussed as a possible order parameter in chapter 9. In the pure gluon theory this is the mass of their lightest bound state, often referred to as a 'glueball.' In principle this quantity appears in a Yukawa law falloff of the correlation between two widely separated sources. Attempts to directly look for such correlations between plaquette operators have been plagued with statistical errors (Bhanot and Rebbi, 1981). Indeed, this correlation becomes swamped by the thermal fluctuations for a separation exceeding only a few lattice spacings. This problem can be circumvented with a combination of a variational method with the Monte Carlo analysis. For the plaquette–plaquette correlation at a short separation of only one or two sites, more than just exchange of the lightest state will be important. This means that a fit to a Yukawa law falloff will give an upper bound on the glueball mass. Using a linear combination of simple operators, for example loops of perimeter up to six links, and finding that combination that minimizes the falloff of the correlation with separation, one can improve the upper bound to a reliable estimate. Effectively, one is attempting to construct an operator which projects the desired state out of the spectrum. This analysis is usually further simplified by projecting out states of zero momentum. This is easily accomplished with a sum over translations transverse to the correlation distance.

Repeating this analysis for several values of coupling gives the functional dependence of the correlation length measured in lattice units. As with the string tension, one can check for the exponential dependence predicted by the renormalization group. The coefficient of this behavior gives the glueball mass in units of the lattice parameter Λ_0. The use of operators with certain discrete lattice symmetries readily generalizes the method to extract the mass of the lightest state with a given set of quantum numbers.

Several groups have developed this technique for the pure $SU(2)$ and $SU(3)$ theories (Berg, Billoire, and Rebbi, 1982; Berg and Billoire, 1982*ab*; Ishikawa, Schierholz and Teper, 1982). For the lightest state with $SU(3)$ these authors find

$$m/\Lambda_0 = 300\text{–}350. \tag{19.14}$$

In physical units this represents 700–1000 MeV, an experimentally intriguing value, although the effects of mixing with normal quark states are unknown. Going on to other quantum numbers, the above authors suggest extremely rich physics in the 1–2 GeV range.

We now come to a third physical parameter which is relatively easy to extract from the Monte Carlo analysis but more difficult to compare with real experiments. In chapter 3 we noted that a finite time length for the lattice permitted the study of finite physical temperatures in the physical quantum system. Thus using a four-dimensional lattice which is smaller in one direction than the others enables us to study the quantum statistical mechanics of pure non-Abelian gauge fields. Actually, the time dimension of the lattice may be varied in a combination of two ways, one by reducing the number of sites in that direction and the other by changing the timelike lattice spacing by means of a different coupling on timelike plaquettes, as used in the Hamiltonian discussion of chapter 15.

The interest in such finite temperature studies is the expectation of a real phase transition (Polyakov, 1978; Susskind, 1979). At low temperatures we should have the quark-confining vacuum with thermal fluctuations producing a dilute ideal gas of glueballs. At high temperatures, however, the vacuum can fill with a spaghetti of flux tubes. In such a pasta, an extra flux tube from an odd quark would quickly become lost. Thus we expect a transition to an unconfined phase in which quarks can wander freely away from each other.

We can regard our finite time system as representing the classical statistical mechanics of a three-dimensional slab of link variables. The deconfining transition corresponds to the spontaneous breaking of a global symmetry in this model. Consider a spacelike hypersurface passing between the sites of the slab, and consider multiplying each link variable that passes through this surface by an element from the center of the gauge group, for example -1 for $SU(2)$. Any plaquette must pass through the hypersurface an even number of times, equally in the two possible directions, and the extra factors will cancel. The action for the statistical system thus has a global symmetry under the center of the gauge group.

To monitor this symmetry, one can define Wilson loops with a net winding number in the timelike direction on the periodic lattice. The simplest such loop is just the trace of the product of all timelike links associated with a particular three-space position. In our toroidal geometry, such a loop is actually a straight line, a 'Wilson line'. These loops must each pass through the spacelike hypersurface an odd number of times and are thus not invariant under the global symmetry. We thus have an order parameter in the sense that a signal for the deconfining transition is the appearance of a spontaneous 'magnetization' with such loops.

A quarklike source on the lattice would produce a periodic world line along one of these loops. For an isolated quark, the product of link variables along this world line gives the gauge field interaction with the source. A vanishing expectation value for the loop is indicative of an infinite energy for an isolated quark in the confined phase. In contrast, a finite 'magnetization' represents the self energy of the quark in interaction with the gauge field soup.

To see that such a transition might well be expected, temporarily consider the extreme case of a one time-site lattice. The 'Wilson line' degenerates into the trace of the one timelike link at any given site. This link variable essentially degenerates into a spinlike variable. Indeed, for an Abelian group these 'spins' decouple from the spacelike loops and become a nearest-neighbor spin model in the three space dimensions. Such models in general have ferromagnetic transitions. For the non-Abelian case there remains a coupling the timelike and spacelike links, and we are left with a spin-gauge model with a global symmetry which can break spontaneously.

We have been discussing this deconfining transition in the pure glue theory without dynamical quarks. Remarkably, the plasma of flux tubes is sufficiently complicated that it can screen a source carrying a non-trivial representation of the gauge group center. This can never be accomplished with a finite number of gluons, each of which is in the adjoint representation and blind to the center. Note the contrast with an adjoint source, which would be screened in both phases. In the full theory with quark loops, quark pairs can always be 'popped' from the vacuum to screen any source. In this case it is unclear what to use for an order parameter, although presumably the existence of the deconfining transition is stable to the introduction of dynamical quarks.

Several groups have used these 'Wilson lines' to locate the critical temperatures for the pure $SU(2)$ and $SU(3)$ deconfining transitions (McLerran and Svetitsky, 1981; Kuti, Polonyi and Szlachanyi, 1981; Engels, Karsch, Satz and Montvay, 1981; Kajantie, Montonen and Pietarinen, 1981). Varying the bare coupling and the number of time sites, one can compare the dimensionless product of the lattice spacing and the critical temperature with the renormalization group prediction, in analogy to the string tension and mass gap analysis. For $SU(3)$ the observed transition temperature is

$$T_c/\Lambda_0 \approx 90 \tag{19.15}$$

or in physical units

$$T_c \approx 200\,\mathrm{MeV}. \tag{19.16}$$

A peculiar feature of this number is its relative smallness in comparison to the glueball mass estimates. As we are considering the quarkless theory, the lightest states above the vacuum have energies large compared to eq. (19.16). This means that just below the transition temperature the vacuum is quite empty, only a low density of isolated glueballs are excited by thermal fluctuations.

An interesting unsettled question is the order of this transition (Svetitsky and Yaffe, 1982). For $SU(2)$ the symmetry being broken is Z_2 and presumably the transition is second order in analogy to the Ising model. However, for $SU(3)$ we have a Z_3 symmetry and the situation is less clear. Mean field theory for Z_3 systems typically predicts first-order transitions (problem 1 of chapter 14). As three dimensions is above the critical dimensionality for discrete symmetry breaking, this prediction must be considered seriously. Indeed, the simple Z_3 spin model, the three-state Potts (1952) model, does exhibit a first-order transition in three dimensions, although the latent heat is quite small (Blote and Swendsen, 1979). Current Monte Carlo studies of the $SU(3)$ deconfining transition are not yet able to determine its order. This question may have some relevance to the evolution of the very early universe.

Temperatures of the order in eq. (19.16) may be experimentally attainable for short times in heavy ion collisions. The relevance of the above calculations for this case is unclear for two reasons. First, such experiments entail a high quark density, and in the above discussion we considered the pure glue theory. Secondly, this temperature is above, although not by a large factor, a hypothetical maximum temperature of order 140 MeV where large numbers of pions would begin to be produced, consuming further kinetic energy forced into the system (Hagedorn, 1970). Indeed, other phase transitions related to pionic physics and/or chiral symmetry breaking may occur well before deconfinement is attained (Kogut *et al.*, 1982). In any case, temperatures in the few hundred MeV range promise rich physics for future experimental studies.

Up to this point our discussion of Monte Carlo simulation has avoided the question of Fermion fields. This is a rapidly evolving subject and therefore the remainder of this chapter is likely to soon be obsolete. The essential difficulty with including quarks in a numerical treatment is that the corresponding path integral is not an ordinary sum, but rather an intricate linear operation from the space of anticommuting variables into the complex numbers. Indeed, the exponentiated action is an operator and cannot be directly compared with real random numbers.

This problem can be immediately (foolishly?) circumvented by first integrating out the anticommuting variables analytically. As discussed in the chapter on fermionic integration, this gives a determinant when the action is quadratic in the anticommuting variables, as is usually the case in practice. This leaves us with an ordinary integral over the gauge fields, to which straightforward Monte Carlo methods are in principle applicable. The main difficulty with this approach is that the determinant is of an extremely large matrix, the number of rows being the product of the number of sites with the ranges of the spinor index, the internal gauge symmetry index, and the flavor index. For interesting sized systems, this is a many-thousand-dimensional matrix. As the time required to take a determinant of a matrix grows with the cube of its dimension, such direct calculations are prohibitively long. Furthermore, naively this determinant needs to be evaluated each time any gauge link is updated. Thus a simulation would seem to require evaluating an impossible determinant many thousands of times.

The actual situation is somewhat better because of various tricks. The fermionic matrix has an enormous number of zero elements. Because the interaction is local, no elements directly couple distant sites. Changes in a link variable alter only a small fraction of the remaining matrix elements. Considering a Metropolis *et al.* (1953) type of algorithm with a small step size, one can confine oneself to study small changes in a small part of the matrix. This still requires the inverse of the matrix, but as the gauge interaction will have stochastic errors anyway, hopefully one does not need the exact inverse. Approximate methods based on iterative schemes

(Weingarten and Petcher, 1981), Monte Carlo simulation with extra boson fields (Fucito *et al.* 1981; Scalapino and Sugar, 1981), and random walks through the matrix (Kuti, 1982) for finding the inverses of large matrices are under active investigation.

Despite these tricks, the fermionic problem is still extremely intensive in its demands on computer resources. An interesting approximation has been reasonably successful in approximately reproducing the hadronic spectrum (Hamber and Parisi, 1981; Weingarten, 1982; Marinari, Parisi and Rebbi, 1981). Instead of evaluating the determinant many times to allow it to feed back into the gauge field dynamics, this approximation considers the inversion of the fermionic matrix in a gauge field configuration obtained in a simulation of the pure quarkless theory. This determines how a quark would propagate in such a fixed background field. The basic approximation is the neglect of the feedback of the fermions on the gauge field. In perturbation theory, this amounts to the sum over all diagrams without any internal virtual quark loops. In a sense it represents the zero flavor limit.

Taking the expectation value of products of the propagators, one can study the propagation of bound state combinations with various meson or baryon quantum numbers. Neglecting internal loops in such systems amounts to considering only valence quarks and ignoring 'sea' quarks in the simple quark model. The experimental fact that a valence quark picture works fairly well suggests that the approximation may not be unreasonable. Internal loops are responsible for the ω splitting from the ρ meson, a relatively small effect. From a less optimistic point of view, neglecting virtual quark pairs neglects the decay of the ρ meson.

Mass estimates are obtained from the long-distance decrease of the meson and baryon propagators. The calculation begins with two parameters, the bare quark mass and the bare charge, which becomes related to the lattice spacing via the renormalization group. Thus two masses must be used to set these bare parameters. One is usually taken as the pion mass and the other either the Regge slope or the ρ mass. The most surprising result of these calculations is the ability to obtain a pion considerably lighter than the other hadrons with their typical scale of order one GeV. The approximation shows a signal of chiral symmetry breaking with the pion as a Goldstone boson. Note that one usually regards such a particle as a coherent excitation on a vacuum which is a condensate of elementary constituent pairs. To see such an effect while neglecting quark loops in the pion propagator is quite remarkable.

Several other predictions for observables should be available from this valence approximation. One can consider the valence quark propagation through three point vertices to obtain information on magnetic moments, form factors, and decay rates. The main missing feature of the procedure lies in states where strong mixing with pure glue states is important, as expected to be the case for the η and η' mesons.

As mentioned earlier, Monte Carlo work with fermions is rapidly evolving. Hopefully the above discussion of the difficulties with fermionic integration will soon become obsolete as the approaches and computer technology improve.

Problem

1. Derive the connection between the Regge slope and the string tension (eq. 19.11).

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