PRACTICAL INTRODUCTION TO MONTE CARLO OF LATTICE QCD AND ITS APPLICATION TO QUARK GLUON PLASMA*

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The paper presents an introduction to Monte Carlo study of lattice gauge theories. Numerical results of Monte Carlo simulation with quark loops are presented.

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CONTENTS

0. Purpose of this lecture

This lecture is aimed at mainly those who will never try Monte Carlo (MC) study of lattice gauge theories. Lattice MC calculations are numerical experiments. Needless to say, any theorists can use experimental data in his or her research. Why not the data from numerical experiments?

In order to make good use of experimental data, however, it is important to know how experimentalists get and treat with data and to understand what are the difficulties.

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Moreover we know our colleague who never uses a computer can help us in this field where many field theoretical and statistical problems should be clarified [1].

There is nothing original in this lecture except Sections 5 and 8. I will present how to get MC data as plainly as possible. Though this lecture can give you only brief outline of the field and for further and deeper understanding I should recommend you the other reviews [2], this note can be easily read by non-specialists even in an armchair without the other references.

PART I

1. Integral over many-dimensional space [3]

Let us consider a numerical integration over n dimensions,

$$I = \int f(x) dx_1 dx_2 \ldots dx_n. \tag{1.1}$$

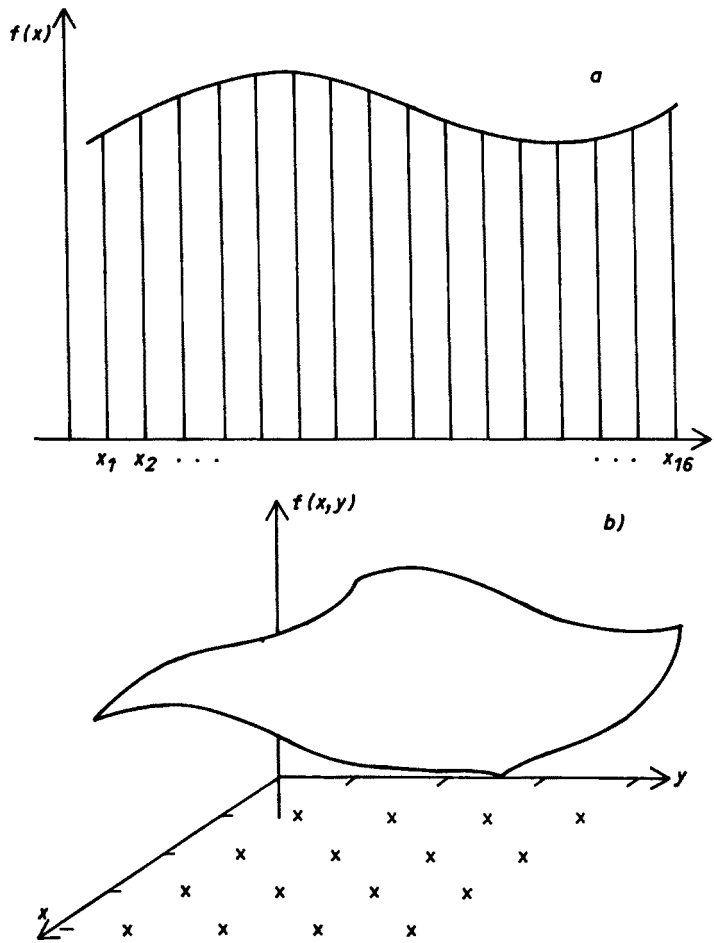


Fig. 1. Function f in n-dimensional space and points where the value of the function is estimated in numerical integration; a) 1-dimension, b) 2-dimensions

Suppose we are so busy that we have only time to evaluate 16 points. For $n = 1$, probably, we can get reasonable approximation (Fig. 1a). For $n = 2$ there are four points in each dimension (Fig. 1b). Perhaps the result is not so reliable. ... For $n = 10$, there are 1.32 points in each dimension. No one believes outcomes of the calculation. If we use the rectangle rule to evaluate Eq. (1), the order of the error is

$$\text{Error} \sim 1/N^{1/n}, \tag{1.2}$$

where N is the number of the total points. (In the above example, $N = 16$.) For very large n, even Simpson rule or Gauss quadrature fails completely to get a reasonable result. In my experiences, it is very hard to calculate Eq. (1.1) if $n > 5$. In case of Lattice QCD n is typically hundred thousands or more.

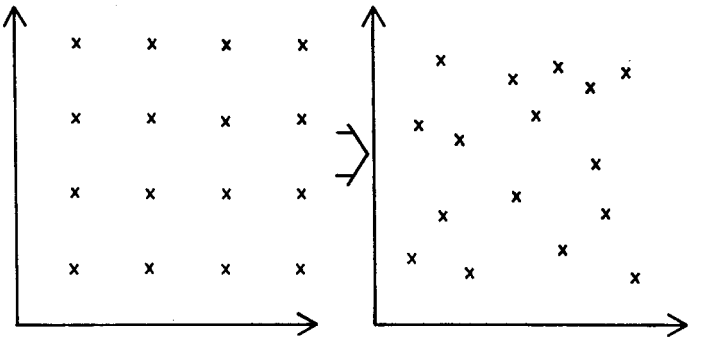


Fig. 2. Numerical integration points distributed uniformly (a) and randomly (b)

In usual quadratures, the points x are chosen regularly in n-dimensional space. On the other hand if we scatter the points randomly in the n-dimensional space (Fig. 2), thanks to the general theorem of statistics, we get

$$\text{Error} \sim 1/\sqrt{N}. \tag{1.3}$$

Note that the dimension of the integration space, n, does not appear in Eq. (1.3), i.e., even for very large n we have a good chance to get accurate results if N is large. This is the essential idea of Monte Carlo method.

The reader may have noticed the accuracy must depend also upon the shape of the function f. If f is nearly flat its integration can be easily done (Fig. 3b), while it is no easy task to integrate a rapidly changing function (Fig. 3a).

Here is a great trick called "Importance Sampling". Let us find a new variable, t, such that

$$\frac{dx}{dt} \sim 1/f. \tag{1.4}$$

Then

$$I = \int f(x(t)) \frac{dx}{dt}\, dt. \tag{1.5}$$

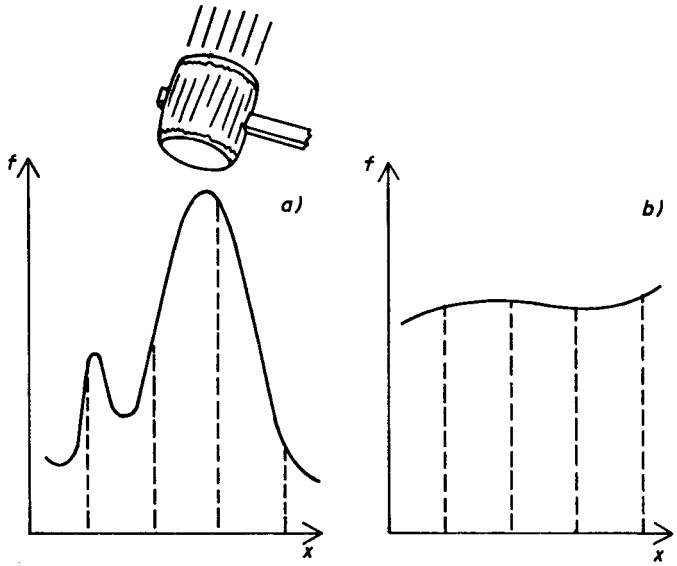


Fig. 3. Rapidly changing function is difficult to integrate numerically (a), while flat function is easy (b). It is nice if we can reform a rapidly changing function to a flat one

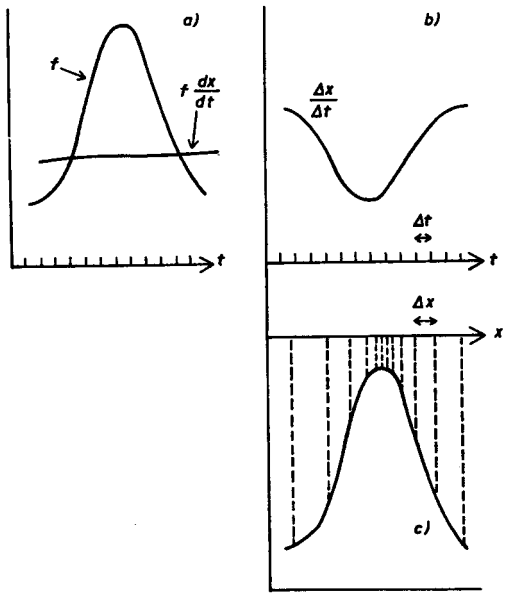


Fig. 4. Shape of a function $f(a)$ and Jacobian $\Delta x/\Delta t$ in Important Sampling (b). If Δt is constant, Δx is large (small) for small (large) Jacobian (c)

Due to condition (1.4), the integrand in Eq. (1.5) is nearly flat. In many cases this simple trick works drastically.

The reader may claim that the idea of importance sampling is clear but it is difficult in general to find such a variable t. Let me go on to investigate this point further. The Jacobian dx/dt is chosen to compensate f, i.e., if f is large, dx/dt is small and vice versa (Figs. 4a and b). If we employ numerical integration method with equi-distance points, i.e., $\Delta t = \text{const.}$, then Δx is small for large f and vice versa (Figs. 4b and c). Therefore the importance sampling method simply means that in x space we should take many points at the regions where $f(x)$ is large (Fig. 4c).

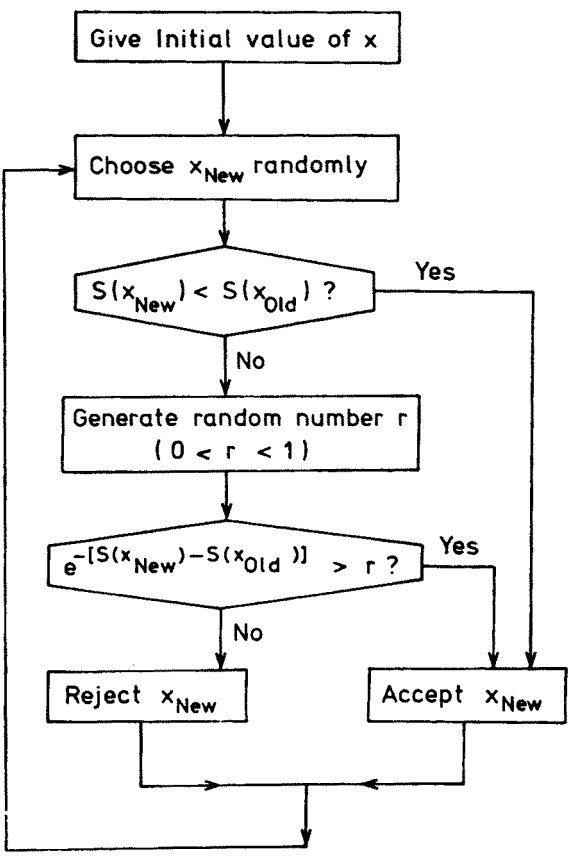
Machinery of choosing points according to the importance sampling is "Metropolis algorithm". Suppose we want to integrate

$$\int e^{-S(x)} dx. \tag{1.6}$$

All that we must do is to choose the points x following a flow chart in Table I. Repeating the procedure, we get many ensembles of the points. We will find the density of the points

TABLE I

Metropolis algorithm



is proportional to exp $(-S)$. I recommend the reader to do Gedankenexperiment for the simple case to see what happens. In Fig. 5 I show a distribution of the points obtained for $S = x^2$.

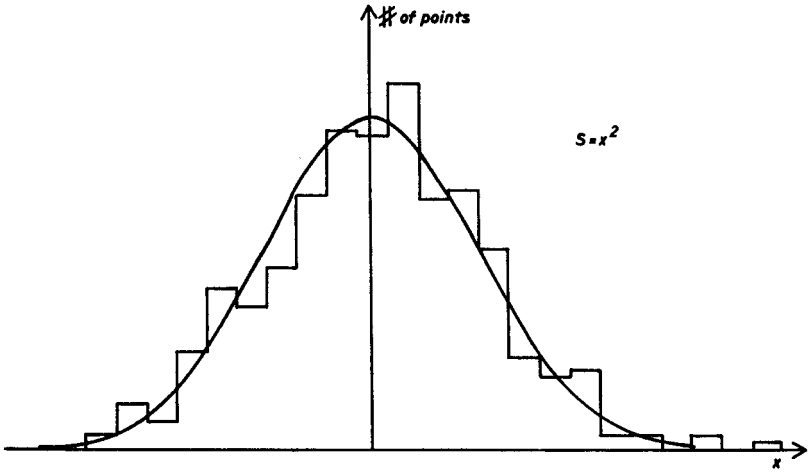


Fig. 5. Distribution of 1000 points obtained by Metropolis algorithm. $S = x^2$. The solid line is the expected behavior (exp $(-x^2)$)

2. *1-dimensional quantum mechanics*

As the simplest example of MC calculations of quantum theory, we will study here one dimensional quantum mechanics [5]. Our system is described by the Feynman path integral,

$$Z = \int \mathcal{D}x e^{\frac{i}{\hbar}\int dt L},$$

$$L = \tfrac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x),$$

$$\mathcal{D}x = \lim_{n\to\infty} dx_1 dx_2 \ldots dx_n. \tag{2.1}$$

Now we go to the Euclidean space,

$$t \to -i\tau,$$

$$L \to -\tfrac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 - V(x) = -H, \tag{2.2}$$

$$Z \to \int \mathcal{D}x e^{-S/\hbar},$$

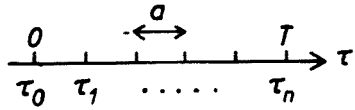
where

$$S = \int d\tau H. \tag{2.3}$$

We cannot go into the real continuum limit in the numerical calculation;

$$Z \simeq \int dx_1\, dx_2 \cdots dx_{n-1}\, e^{-S/\hbar}$$

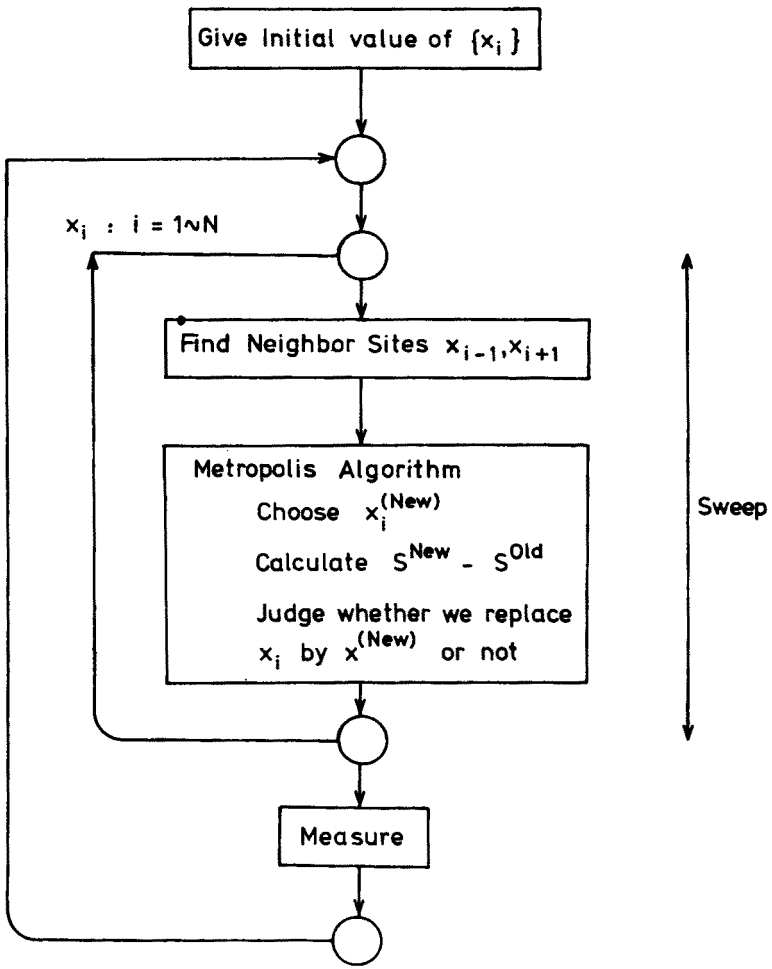
$$x_j = x(\tau_j). \qquad (2.4)$$



$$S = \sum_j a \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{a} \right)^2 + V(x_j) \right]$$

TABLE II

Flow-chart of one dimensional lattice quantum mechanics



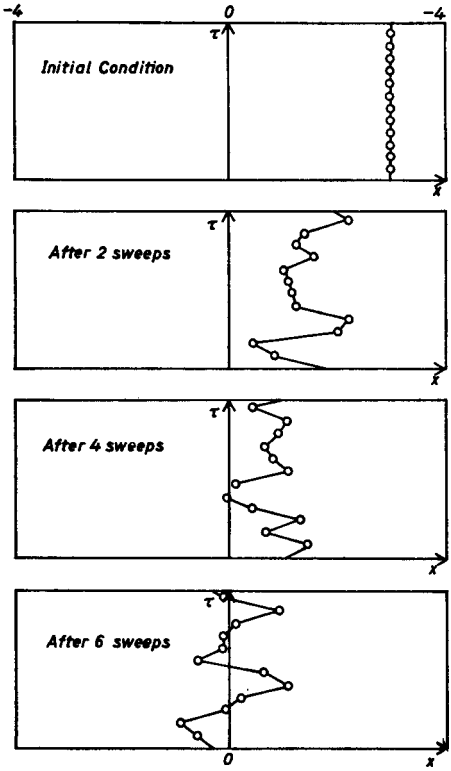


Fig. 6. Behavior of (x_i) after several sweeps when we start far from equilibrium

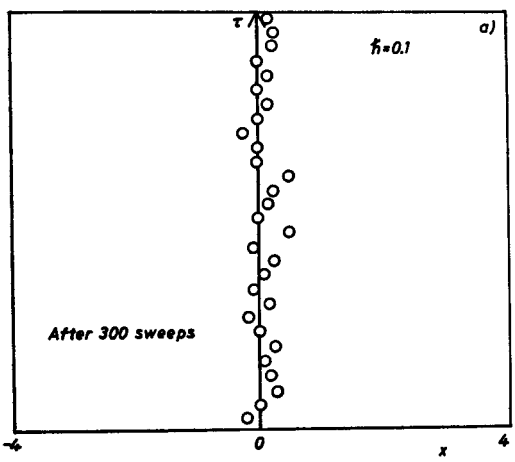


Fig. 7a

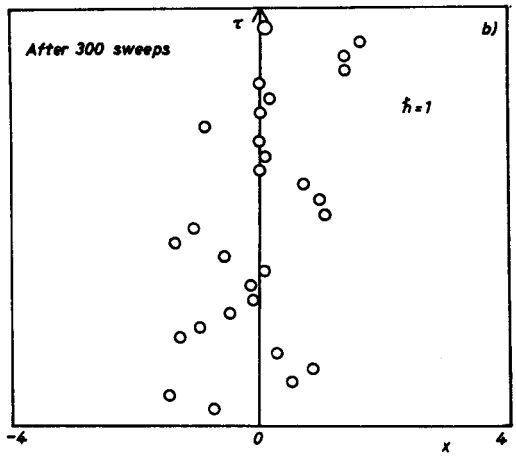


Fig. 7b

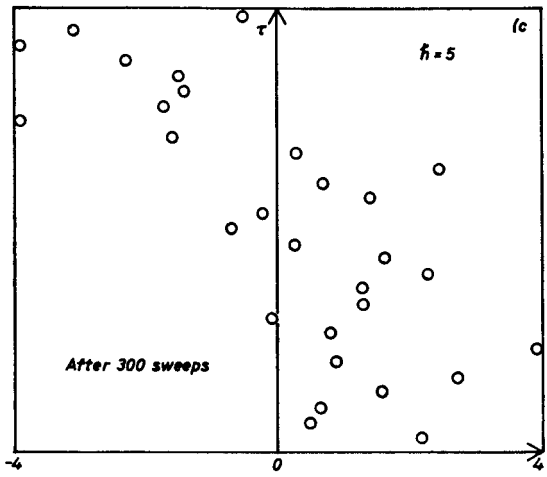


Fig. 7c

Fig. 7. Typical configuration of $\{x_i\}$ for $\hbar = 0.1$ (a), 1 (b) and 5 (c). $V = x^2$

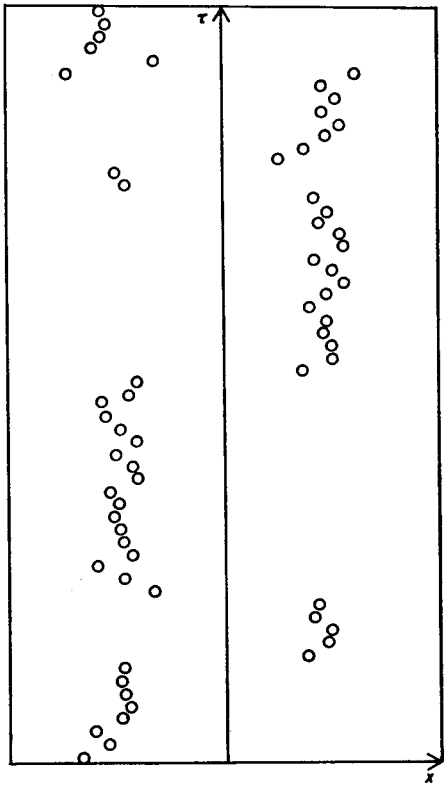


Fig. 8. Typical configurations of x_i for the unharmonic potential $V = 8x^2 + x^4$

Using the MC technique which we learned in the previous Section, we are now able to evaluate Eq. (2.4). In Table II a flow chart of the program is presented. Note that when we estimate the difference of the action

$$S^{\text{new}} - S^{\text{old}} = S(\ldots x_i^{(\text{new})} \ldots) - S(\ldots x_j^{(\text{old})} \ldots),$$

we need not calculate the full part of S because most parts of the action are the same between $S^{(\text{new})}$ and $S^{(\text{old})}$. One procedure to update all x_i is called a sweep. In Fig. 6, I show how quickly the configuration $\{x_i\}$ is going to the equilibrium even when it starts far from equilibrium. Figs. 7a, b and c show the typical configurations for three different values of the Plank constant, $\hbar = 0.1$, 1 and 5. Fig. 8 is the typical configuration for double minimum (wine bottle) potential.

3. *Lattice QCD Lagrangian*

In the lattice QCD, the Eulidean space-time is approximated by a four-dimensional lattice, whose element is usually a hyper-cube, and the quarks and gluons live on its sites and linkes, respectively. See Fig. 9. Integration measure of the path integral is replaced by the integration over such variables:

$$\mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi \to \Pi\, dU_{n,m} \Pi\, d\bar{\psi}_n d\psi_n. \tag{3.1}$$

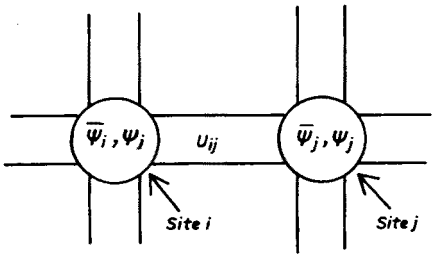
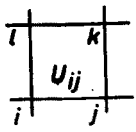


Fig. 9. Gluonic variables live at links and quark variables at sites on a lattice

Wilson has given the lattice action as [6]



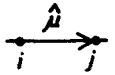
$$S = S_G + S_F,$$

$$S_G = \beta \sum_{\text{plaq}} \left\{1 - \frac{1}{N} \mathrm{Tr}\,(U_{ij} U_{jk} U_{kl} U_{li})\right\}, \tag{3.2}$$

$$\beta = 2N/g^2,\ U_{ij} \in SU(N),$$

$$S_F = \sum_{ij} \bar{\psi}_i \Delta(i,j) \psi_j,$$

where



$$\Delta(i,j) = 1 - \kappa \sum_{\mu=1}^{4} \left\{(1-\gamma_\mu) U_{ij}\ \delta_{i+\hat{\mu},j} + (1+\gamma_\mu) U_{i,j}\ \delta_{i-\hat{\mu},j}\right\}$$

Here I suppress the color indices of U (do not confuse i and j with color matrix indices) and the color, flavor and Dirac indices of ψ. The gluon link variables, U, and the quark site variables, ψ, are related to their corresponding continuum field variables as

$$U_{n,n+\hat{\mu}} = e^{igaA_\mu(na)}, \qquad \psi_n = \sqrt{\frac{a^3}{2\kappa}}\,\psi(na). \tag{3.3}$$

Using these relations one can easily find that *classical* continuum limits of S_G and S_F are familiar QCD actions:

$$\lim_{a\to 0} S_G = \tfrac{1}{2}\int d^4x\ \mathrm{Tr}\,\{F_{\mu\nu}^2\},$$

$$\lim_{a\to 0} S_F = -\int d^4x\{m\bar{\psi}(x)\psi(x)+\bar{\psi}(x)\gamma_\mu(\partial_\mu+igA_\mu)\psi(z)\}, \tag{3.4}$$

if we set a hopping parameter, κ, as

$$\kappa = \frac{1}{8+2ma}. \tag{3.5}$$

Gauge transformation on a lattice is rather simple:

$$\psi_n \to \omega_n\psi_n,\ \bar{\psi}_n \to \bar{\psi}_n\omega_n^\dagger,$$

$$U_{nm} \to \omega_n U_{nm}\omega_m^\dagger, \qquad U_{nm},\ \omega_n \in \mathrm{SU}(N). \tag{3.6}$$

Under this transformation the following expressions are invariant, $U_{ij}U_{jk}\ldots U_{ni}$, $\bar{\psi}_i U_{ij}U_{jk}\ldots U_{mn}\psi_n$. Therefore the action (3.1) is gauge-invariant. In the continuum limit we can easily get

$$\psi(x) \to \omega(x)\psi(x), \qquad \bar{\psi}(x) \to \bar{\psi}(x)\omega(x)^\dagger,$$

$$A_\mu(x) \to \omega(x)A_\mu(x)\omega(x)+\frac{i}{g}(\partial_\mu\omega(x))\omega(x)^\dagger.$$

Young students should check the relations (3.4) all by themselves. The answer may be found, for example, in the appendix of Ref. [6b]. Through this exercise, they may find more general form for the fermionic part:

$$\Delta = cI-\kappa\sum_\mu\{(r-\gamma_\mu)U_{ij}\delta_{i+\hat{\mu},j}+(r+\gamma_\mu)U_{ij}\delta_{i-\hat{\mu},j}\}, \tag{3.7}$$

$$\kappa = \frac{c}{8r+2ma}.$$

The r is called Wilson term.

They may notice also that the lattice distance in spacial directions, a_l, is not necessarily equal to that in temporal direction, a_t. For such an asymmetric lattice,

$$1-\frac{1}{2N}\mathrm{Tr}\,(UUUU)\to\begin{cases}a_l^4\beta\,\mathrm{Tr}\,(F_{kl}^2) & \text{for a spacial plaquette}\\ a_t^2a_l^2\beta\,\mathrm{Tr}\,(F_{tl}^2) & \text{for a temporal plaquette}\end{cases} \tag{3.8}$$

$$\psi_n\to\sqrt{\frac{a_l}{2\kappa_t}}\,\psi(na),$$

and

$$\kappa_t=\frac{1}{2ma_t+(2+6a_t/a_l)r}, \tag{3.9}$$

$$\kappa_l=\frac{1}{2ma_l+(2a_l/a_t+6)r}.$$

The reader may wonder why we need the Wilson term, r, which disappears when we take the continuum limit. This is probably the most challenging, difficult and annoying problem in lattice gauge theories with fermions [7]. Analysis of this problem requires another lecture note (and another lecturer). Here I will not discuss this problem. I only recall that S_F can be diagonalized if $r=0$ [8].

If we put r to be zero, the fermion action has the form;

$$S_F=2ma\bar\psi_n\psi_n+\sum_\mu\{\bar\psi_n\gamma_\mu U_{n,n+\hat\mu}\psi_{n+\hat\mu}-\bar\psi_{n+\hat\mu}\gamma_\mu U_{n+\hat\mu,n}\psi_n\}, \tag{3.10}$$

where we put c to be $2ma$. We introduce the following (local) unitary transformation,

$$\psi_n=T_n\chi_n,\ \bar\psi_n=\bar\chi_nT_n^\dagger$$

$$T_n=(\gamma_1)^{n_1}(\gamma_2)^{n_2}(\gamma_3)^{n_3}(\gamma_4)^{n_4},\qquad n=(n_1,n_2,n_3,n_4). \tag{3.11}$$

It is easy to check

$$\bar\psi_n\gamma_1\psi_{n+\hat1}=\bar\chi_n(\gamma_4)^{n_4}(\gamma_3)^{n_3}(\gamma_2)^{n_2}(\gamma_1)^{n_1}\gamma_1(\gamma_1)^{n_1+1}(\gamma_2)^{n_2}(\gamma_3)^{n_3}(\gamma_4)^{n_4}\chi_{n+\hat1}=\bar\chi_n\chi_{n+\hat1},$$

$$\bar\psi_n\gamma_2\psi_{n+\hat2}=(-1)^{n_1}\bar\chi_n\chi_{n+\hat2},$$

$$\bar\psi_n\gamma_3\psi_{n+\hat3}=(-1)^{n_1+n_2}\bar\chi_n\chi_{n+\hat3},$$

$$\bar\psi_n\gamma_4\psi_{n+\hat4}=(-1)^{n_1+n_2+n_3}\bar\chi_n\bar\chi_{n+\hat4}.$$

Then

$$S_F=2ma\bar\chi_n\chi_n+\sum_\mu\eta_\mu(n)\{\bar\chi_nU_{n,n+\hat\mu}\chi_{n+\hat\mu}+\bar\chi_{n+\hat\mu}U_{n+\hat\mu,n}\chi_n\}, \tag{3.12}$$

where

$$\eta_\mu(n)=\begin{cases}1(\mu=1), & (-1)^{n_1}(\mu=2),\\ (-1)^{n_1+n_2}(\mu=3), & (-1)^{n_1+n_2+n_3}(\mu=4).\end{cases}$$

There is no γ matrix! χ is essentially one component in Dirac index space. We call this Susskind action. This action is convenient when we want to say something about the chiral symmetry, while a hadron wave function is complicate: it is not local but constructed from quarks on 16 vertices of a hyper-cube. Detailed analyses can be found in Ref. [9].

4. Lattice gauge theories without fermion

There are too many works about this topic in the literatures. I will discuss here only some of them which will be helpful in Part II.

Anyhow we want to measure something;

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}U \mathcal{O} e^{-S}}{\int \mathcal{D}U e^{-S}} . \tag{4.1}$$

In a MC calculation, the configuration $\{U\}$ is generated according to the probability $\exp(-S)$. Therefore the expectation value of $\mathcal{O}$ is obtained simply as a mean:

$$\langle \mathcal{O} \rangle = \sum_k \mathcal{O}^{(k)} / \sum_k \tag{4.2}$$

where $\mathcal{O}^{(k)}$ is the value of the operator $\mathcal{O}$ in the k-th configuration.

A. Wilson loop and Polyakov line

Observable quantities should be gauge invariants. Without quarks the simplest ones are the Wilson loop, W, and the Polyakov line, L. For SU(N) they are defined as

$$W = \frac{1}{N} \mathrm{Tr}\,(U_{ij} U_{jk} \cdots U_{li}), \tag{4.3}$$

$$L = \frac{1}{N} \mathrm{Tr}\,(U_{12} U_{23} \cdots U_{n-1n}).$$

Sometimes they are defined without a factor N. See Fig. 10. If all link variables are the same on a lattice (frozen), $L = 1$; if completely random, $\langle L \rangle = 0$.

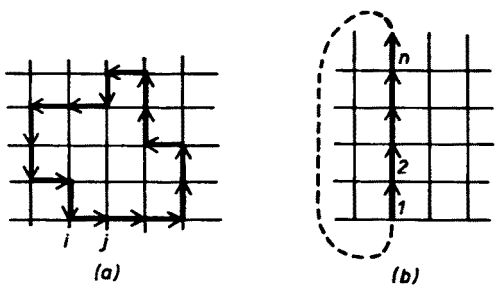


Fig. 10. Wilson loop (a) and Polyakov line (b)

Let us consider the physical meaning of the Wilson line and Polyakov line briefly. Suppose an external source, $j_\mu = g\delta^3(x_\mu - x_\mu(t))$, is added to the system. The total energy of the system is increased by

$$i\int d^4x j_\mu A_\mu = ig\int dx_\mu A_\mu,$$

and the action is modified,

$$e^{-S_G} \to e^{ig\int dx_\mu A_\mu - S_G} = e^{igaA_n} e^{igaA_{n-1}} \cdots e^{igaA_1} e^{-S_G}. \tag{4.4}$$

Therefore if we calculate the expectation value of $L \times T$ Wilson loop, we can estimate the potential between external sources, i.e., infinitely heavy quarks,

$$\left\langle Tr\left(\square\right)\right\rangle = \frac{Z \text{ with } \square}{Z}$$

$$= e^{-TV(L)} \tag{4.5}$$

Stack has obtained an impressive shape of the heavy quark potential from Wilson loop data [10]. See Fig. 11.

The expectation value of a Polyakov line should be zero in a confined phase.

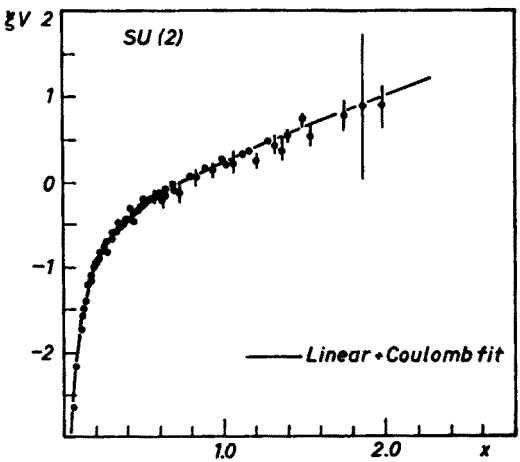


Fig. 11. Heavy quark potential obtained by Stack

B. Lattice distance, a, is a function of β

In Fig. 12 we show the famous MC measurement of the string tension, σ, by Creutz as a function of $\beta(=2N/g^2)$ [11]. We observe rapid decreasing of $a^2\sigma$, i.e., the lattice distance, a, changes very quickly as β increases. We may see this trend both from the pertur-

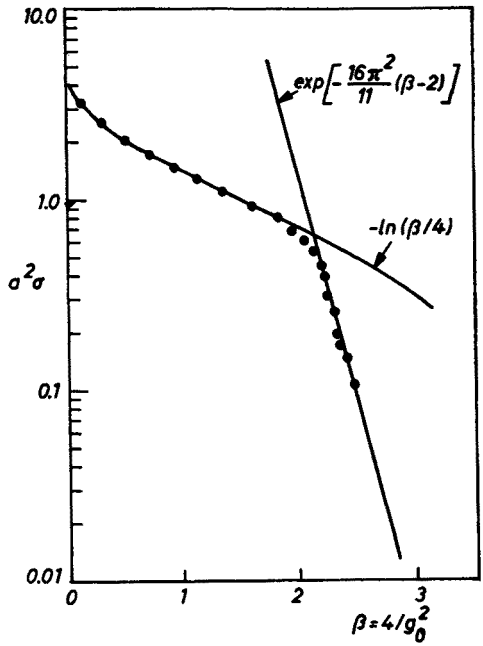


Fig. 12. String tension obtained by Creutz as a function of $\beta = 4/g^2$

bation and the strong coupling expansion. From dimensional analysis, we can write

$$m = \frac{1}{a} F(g), \tag{4.6}$$

where m is some physical quantity which has mass dimension. Any physical quantity must be independent of the cut off which is π/a in lattice theories,

$$\frac{d}{da} m = 0. \tag{4.7}$$

We substitute Eq. (4.6) into Eq. (4.7) and get

$$F = a \frac{dF}{da} = a \frac{dg}{da} \frac{dF}{dg} = -\beta(g) \frac{dF}{dg}, \tag{4.8}$$

where $\beta(g)$ is the β function (which has nothing to do with the coupling $\beta = 2N/g^2$),

$$\beta = -\beta_0 g^3 - \beta_1 g^5 + \ldots . \tag{4.9}$$

If we neglect the higher terms in the β function, we find

$$F = cf(g) \quad \text{or} \quad m = \frac{c}{a} f(g), \tag{4.10}$$

where c is a constant and

$$f(g) = \exp\left(-\frac{1}{2\beta_0 g^2}\right)\left(\frac{1}{\beta_0 g^2}\right)^{\frac{\beta_1}{2\beta_0^2}}. \tag{4.11}$$

Therefore

$$a = \frac{c}{m} f(g) = \frac{1}{\Lambda} f(g). \tag{4.12}$$

The student should derive Eq. (4.11) from Eqs. (4.6)–(4.9).

We give here the perturbative results of the β function coefficients [12];

$$\beta_0 = \frac{1}{(4\pi)^2}\left(\tfrac{11}{3} N_c - \tfrac{2}{3} N_f\right),$$

$$\beta_1 = \frac{1}{(4\pi)^4}\left(\tfrac{34}{3} N_c^2 - \tfrac{10}{3} N_c N_f - \frac{N_c^2 - 1}{N_c} N_f\right). \tag{4.13}$$

In Fig. 13, I show the behavior of $f(g)$.

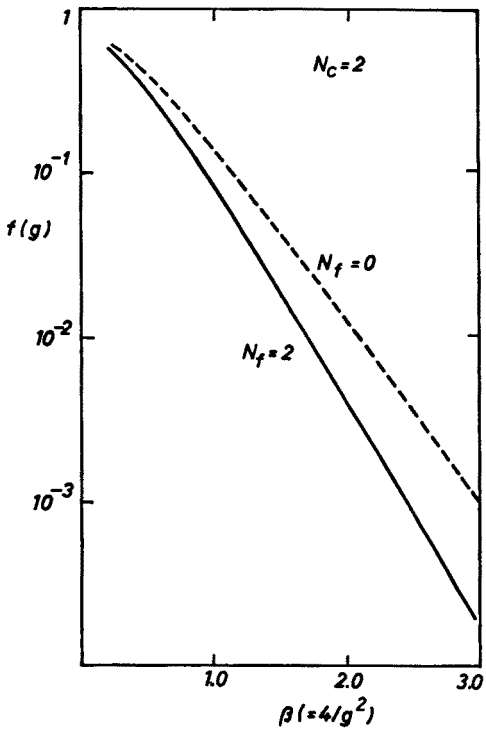


Fig. 13. Behavior of a function $f(g)$ for pure gauge case ($N_f = 0$) and for 2 flavour case. For the definition of f, see the text

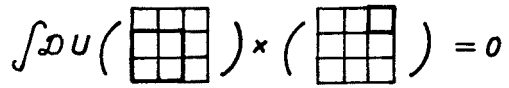
Next we study the behavior of a from the strong coupling expansion. Formula which we need is only

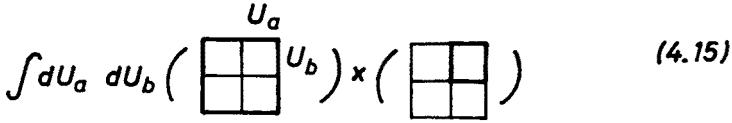
$$\int dU = 1,$$

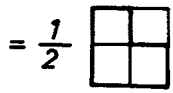
$$\int dU(U)_{\alpha\beta} = \int dU(U^\dagger)_{\alpha\beta} = 0,$$

$$\int dU(U)_{\alpha\beta}(U^\dagger)_{\gamma\delta} = \tfrac{1}{2}\,\delta_{\alpha\delta}\delta_{\beta\gamma}. \tag{4.14}$$

Using these group integrals, we can find



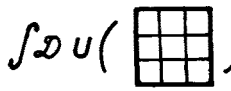


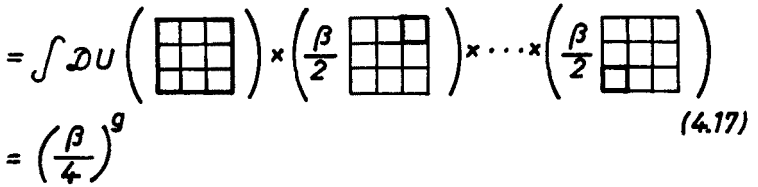


We rewrite

$$e^{-S_G} = C\Pi e^{\frac{1}{2}\beta\,\mathrm{Tr}\,UUUU} = C(1+\beta\,\mathrm{Tr}\,UUUU+\ldots) \tag{4.16}$$

Then





We can easily guess a form of the expectation value of $N_t \times N_1$ Wilson loop:

$$\langle W\rangle \simeq \left(\frac{\beta}{4}\right)^{N_t N_1} = e^{-\frac{TL}{a^2}\log\frac{4}{\beta}}. \tag{4.18}$$

From Eq. (4.18) we get

$$V(L) = \sigma L, \quad \sigma = \frac{1}{a^2}\log\frac{4}{\beta}. \tag{4.19}$$

The string tension, σ, should be independent of β. The lattice distance, therefore, behaves as

$$a \sim \sqrt{\log 4/\beta}. \tag{4.20}$$

Now we know that when β is large a is small, i.e., we are near to the continuum. Why do we not perform MC calculation at very large β? Unfortunately the lattice size is finite. Therefore if a is very small the lattice length is also small. See Fig. 14. The lattice

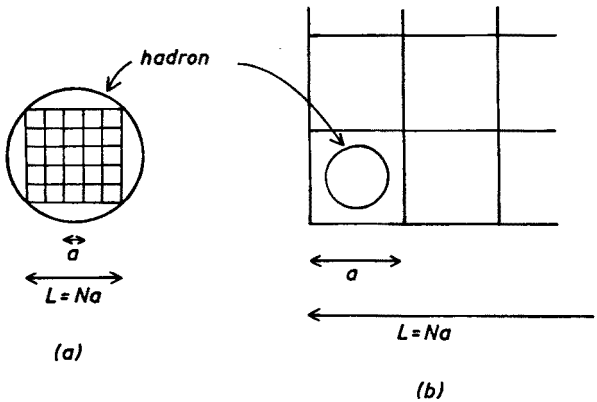


Fig. 14. a) If the lattice distance a is very small, the lattice itself is smaller than typical hadronic size. b) If the lattice distance a is very large, it is larger than typical hadronic size. Both cases are disaster

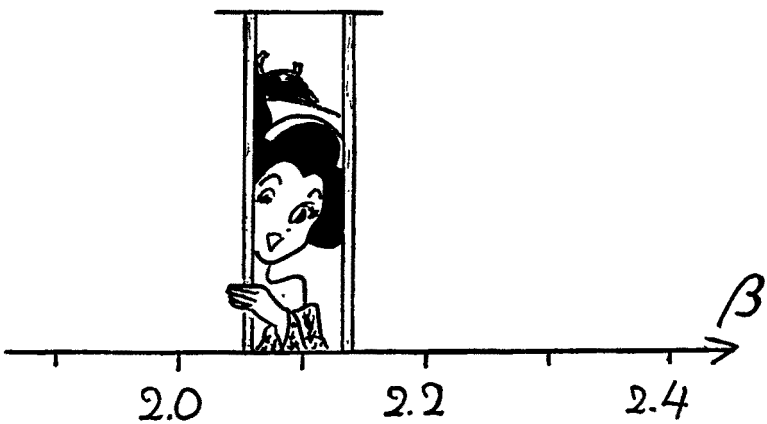


Fig. 15. Window in β for SU(2)

distance should be small enough to describe hadron physics well but should be so large that the lattice is larger than hadron size. It was believed that there is a window in β where these two conditions are satisfied; $\beta = 2.1 \sim 2.2$ for SU(2) (Fig. 15). However recent measurement of the string tension casts some doubt upon this folklore. See Table III.

TABLE III

String tension in SU (2) obtained on lattices of different size and by different groups

	Authors	$\sqrt{\sigma}/\Lambda$	Lattice	Ref.
1	M. Creutz	200 ± 50	4^4, 6^4	*Phys. Rev. Lett.* **45**, 313 (1980)
2	F. Gutbrod et al.	$<145\pm 10$	16^4	*Phys. Lett.* **128B**, 415 (1983)
3	G. Parisi et al.	85 ± 5	$10^3\times 20$	*Phys. Lett.* **128B**, 418 (1983)

5. Lattice gauge theories with fermion

In the path integral, the fermion fields appear as a Grassman variable, i.e., anti-commuting c-number [13]:

$$\begin{aligned}\bar{\psi}_i\psi_k+\psi_k\bar{\psi}_i &= \delta_{ik},\\ \bar{\psi}_i\bar{\psi}_k+\bar{\psi}_k\bar{\psi}_i &= 0,\\ \psi_i\psi_k+\psi_k\psi_i &= 0.\end{aligned} \tag{5.1}$$

The rules of integration devised by Berezin are

$$\begin{aligned}\int d\bar{\psi}_i &= \int d\psi_i = 0,\\ \int \bar{\psi}_i d\bar{\psi}_i &= \int \psi_i d\psi_i = 1.\end{aligned} \tag{5.2}$$

It is easy to show

$$\int \exp\Big(\sum_{i,j=1}^{2} \bar{\psi}_i A_{ij}\psi_j\Big) d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 = A_{11}A_{22}-A_{12}A_{21} = \det A.$$

General form is known as Matthews-Salam formula;

$$\begin{aligned}\int \mathscr{D}\bar{\psi}\mathscr{D}\psi e^{\bar{\psi}A\psi} &= \det A,\\ \int \mathscr{D}\bar{\psi}\mathscr{D}\psi(\bar{\psi}_i\psi_j)e^{\bar{\psi}A\psi} &= (A^{-1})_{ji}\det A,\\ \int \mathscr{D}\bar{\psi}\mathscr{D}\psi(\bar{\psi}_i\psi_j\bar{\psi}_k\psi_l)e^{\bar{\psi}A\psi} &= \{(A^{-1})_{ji}(A^{-1})_{lk}-(A^{-1})_{jk}(A^{-1})_{li}\}\det A.\end{aligned} \tag{5.3}$$

We can, therefore, integrate over fermion degrees of freedom,

$$\begin{aligned}Z &= \int \mathscr{D}U\mathscr{D}\bar{\psi}\mathscr{D}\psi e^{-S_G-\bar{\psi}\Delta\psi} = \int \mathscr{D}U \det\Delta e^{-S_G},\\ \langle\bar{\psi}_i\psi_j\rangle &= \int \mathscr{D}U(\Delta^{-1})_{ji}\det\Delta e^{-S_G},\ \ldots\end{aligned} \tag{5.4}$$

How can we take into account det Δ. Surely the simplest way is so-called quenched approximation where this determinant is discarded:

$$\det\Delta = 1. \tag{5.5}$$

As we will see later, the physical meaning of Eq. (5.5) is neglecting quark loops. An excuse for this approximation is that OZI violation is small and the valence quark picture is not

so bad. Hadron masses and magnetic moments have been measured under this condition and acceptable results have been obtained [14].

But is this really good assumption? In other words, does det Δ depend upon gauge configurations so weakly? Joos and Montovey performed an interesting experiment about this problem. They calculated $S_{\text{E.F.}}$ on 20 samples of gauge configuration where $S_{\text{E.F.}}$ is an effective fermion action,

$$\det \Delta = e^{-S_{\text{E.F.}}}. \tag{5.6}$$

The result is shown in Fig. 16 as a function of the hopping parameter, κ. The observed large deviation of $S_{\text{E.F.}}$ implies that, if gauge configurations are generated according to the

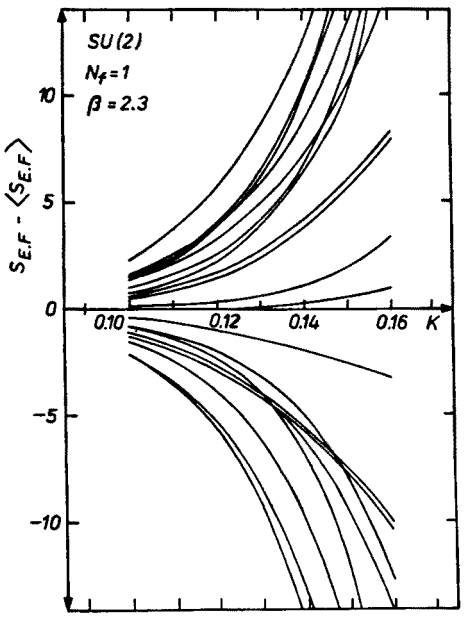


Fig. 16. Behaviour of $S_{\text{E.F.}}$ as a function of a hopping parameter. (H. Joos, I. Montvay, *Nucl. Phys.* **B225** (FS9), 565 (1983))

probability $\exp(-S_G)$, $\det \Delta \exp(-S_G)$ is very small for many of the configurations. Recalling the idea of the importance sampling to our mind, we should generate gauge configurations according to the probability

$$\det \Delta e^{-S_G} = e^{-S_G - S_{\text{E.F.}}}. \tag{5.7}$$

Several ways have been proposed to take into account the quark loops;

A. Hopping parameter expansion (HOPE) [15]

Notice that Δ can be written as

$$\Delta = I - \kappa M. \tag{5.8}$$

Formally we can expand $S_{\text{E.F.}}$ and Δ^{-1} in a series of κ:

$$S_{\text{E.F.}} = -\log\det\Delta = -\mathrm{Tr}\log(I-\kappa M) = \sum_l \frac{\kappa^l}{l}\mathrm{Tr}\,M^l, \tag{5.9}$$

$$\Delta^{-1} = \sum_l \kappa^l M^l.$$

Recall that M includes the Kronecker delta which connects neighboring sites. We can check $\mathrm{Tr}(M^k) \neq 0$ only if M^k draws a closed loop whose length is k (Fig. 17).

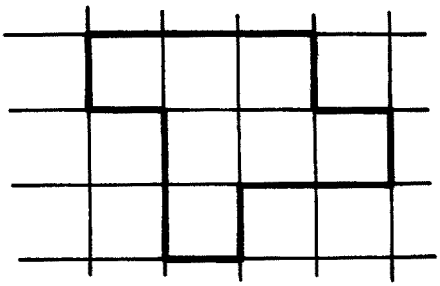


Fig. 17. A typical quark loop

B. Pseudo-fermion method [16]

This method is based on the following observation. If we introduce an average over new bosonic fields, ϕ, which have the same degrees of freedom as ψ (Dirac, color, flavor and sites indices),

$$\bar{\mathcal{O}} = \frac{\int \mathcal{D}\phi^*\mathcal{D}\phi\mathcal{O}e^{-S_\phi}}{\int \mathcal{D}\phi^*\mathcal{D}\phi e^{-S_\phi}},$$

$$S_\phi = \langle\chi|\chi\rangle, \tag{5.10}$$

$$|\chi\rangle = \Delta|\phi\rangle,$$

then the Δ^{-1} is given by

$$\Delta^{-1} = \overline{|\phi\rangle\langle\chi|}. \tag{5.11}$$

The ϕ are called pseudo fermion fields. The integral (5.10) is estimated by MC method. In this calculation all the elements of Δ^{-1} are obtained at the same time.

In the Metropolis algorithm to update the gauge fields we need

$$\delta S = \delta S_{\text{G}} + \delta S_{\text{E.F.}}. \tag{5.12}$$

For small change of the gauge configuration,

$$\delta S_{\text{E.F.}} = -\mathrm{Tr}(\Delta^{-1}\delta\Delta). \tag{5.13}$$

C. Microcanonical method [17]

In addition to the gauge variable, U, let us introduce *classical* fields, ϕ and new time t which has nothing to do with the real time. Imagine a classical system governed by a Lagrangian,

$$L = -S_G + \tfrac{1}{2}\left(\frac{dU}{dt}\right)^2 + \left(\frac{d\phi^*}{dt}\right)\Delta\left(\frac{d\phi}{dt}\right) - \omega^2\phi^*\phi. \tag{5.14}$$

The corresponding Hamiltonian is

$$H = \tfrac{1}{2}p^2 + P\Delta^{-1}P^* + S_G + \omega^2\phi^*\phi, \tag{5.15}$$

where p and P are the conjugate momenta of U and ϕ. The partition function of the classical system is

$$Z = \int \mathcal{D}U\mathcal{D}p\mathcal{D}\phi\mathcal{D}\phi^*\mathcal{D}P\mathcal{D}P^* e^{-H/\vartheta} = c\int \mathcal{D}U \det\Delta e^{-S_G/\vartheta}. \tag{5.16}$$

This is just the form that we want to evaluate. If we accept the Ergodic Hypothesis, we may replace ensemble average with time average. Equations of motion of the system are

$$\begin{aligned} p &= \frac{dU}{dt}, \qquad P = \left(\frac{d\phi^*}{dt}\right)\Delta, \\ \frac{d^2U}{dt^2} &= -\frac{dS_G}{dU} + \frac{d\phi^*}{dt}\frac{d\Delta}{dU}\frac{d\phi}{dt}, \\ \frac{d}{dt}\left(\frac{d\phi^*}{dt}\Delta\right) &= -\omega^2\phi^*. \end{aligned} \tag{5.17}$$

If we follow the trajectory obtained by Eqs. (5.17) and calculate time average of some quantity on the trajectory, the effect of $\det\Delta$ is automatically included.

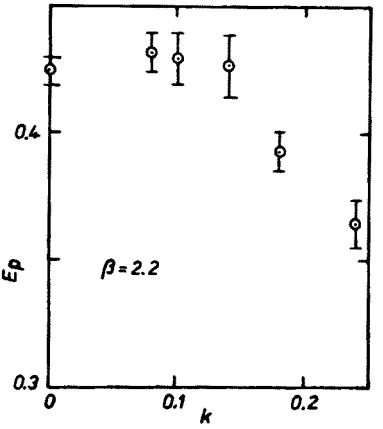


Fig. 18. Expectation value of the plaquette energy as a function of the hopping parameter ($\kappa = 0$ corresponds to the pure gauge case)

TABLE IV

Compilation of MC experiments with quark loops

Authors	Color Lattice	Method Action	Observed quantities
V. Azcoiti, A. Nakamura and A. Cruz[1]	SU(2) 4^4, $(4^3 * 8)$	Pseudo-Ferm. Wilson Act.	E_p, $\langle L \rangle$, $\langle E_p^2 \rangle - \langle E_p \rangle^2$ Meson Masses
H. Hamber, E. Marinari, G. Parisi and C. Rebbi[2]	SU(3) 6^4	Pseudo-Ferm. Susskind Act.	E_p
S. Otto[3]	SU(3) 2^4	Pseudo-Ferm	E_p
I. Montvay[4]	SU(2) 10^4	32-HOPE Wilson Act.	Meson Masses
I. Montvay[5]	SU(3) 6^4	16-HOPE Wilson Act.	Wilson Loops

[1] *Phys. Rev.* **D27**, 255 (1983); Frascati preprint LNF-84/25.
[2] *Phys. Lett.* **124B**, 99 (1983).
[3] *Phys. Lett.* **135B**, 129 (1983).
[4] *Phys. Lett.* **132B**, 393 (1983).
[5] *Phys. Lett.* **139B**, 70 (1984).

I compile MC experiments with quark loops in Table IV where finite temperature calculations are not included. (They will be discussed in Part II.) Present situation is far from satisfactory. We have not yet perfomed a good experiment with high statistics on a large lattice. It seems, however, such MC experiment is now within our scope.

I will mention some general features of the present data. I plot the expectation value of the plaquette energy, E_p, as a function of κ, in Fig. 18, where the point at $\kappa = 0$ cor-

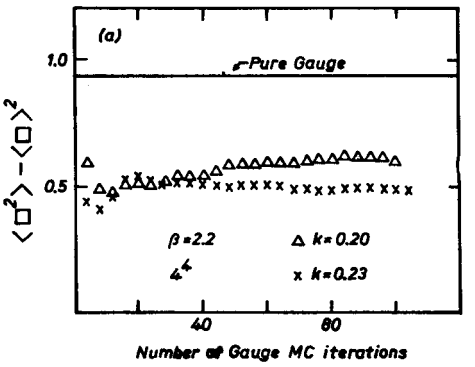


Fig. 19. Fluctuation of the plaquette energy against the number of MC gauge sweeps. The solid line stands for the pure gauge case. The values are scaled up by 10^3

responds to the pure gauge case. When we put quark loops into the system, the plaquette energy decreases; the gauge configuration becomes more ordered state. This tendency can be seen also in Fig. 19 where the fluctuation of the plaquette energy is shown to be smaller than that of the pure gauge case. In Fig. 20 we compare the expectation value of $S_{\text{E.F.}}$ with that of S_{G}. There is a sizable contribution of det Δ to the total action at large κ, i.e., light quark mass regions.

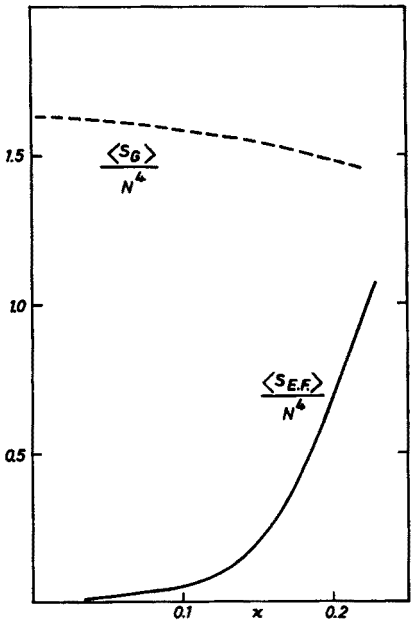


Fig. 20. Expectation value of $S_{\text{E.F.}}$ and S_{G} as a function of the hopping parameter

PART II

6. World at high temperature and high density

It has been conjectured that systems of quarks and gluons at high temperature and density show completely different behavior from those at zero temperature and normal density. For more detailed arguments and references see Refs [1]. At low temperature and low chemical potential, quarks and gluons are confined inside hadrons (Fig. 21a). If hadronic spectrum increases exponentially,

$$\varrho(m) = Ce^{m/T_0} \tag{6.1}$$

a partition function diverges above some temperature T_0;

$$\int dm\varrho(m)e^{-m/T} = \infty \quad \text{if} \quad T > T_0. \tag{6.2}$$

This observation leads to famous limiting temperature a la Hagedorn. Cabibbo and Parisi have shown that this break-down of the partition function does not necessarily

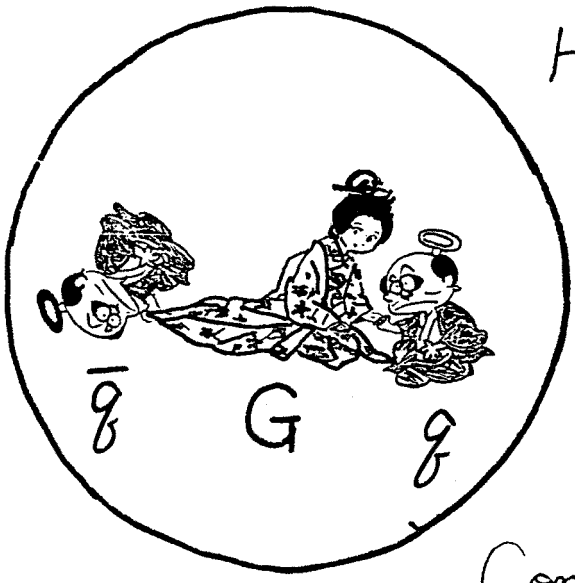


Fig. 21a

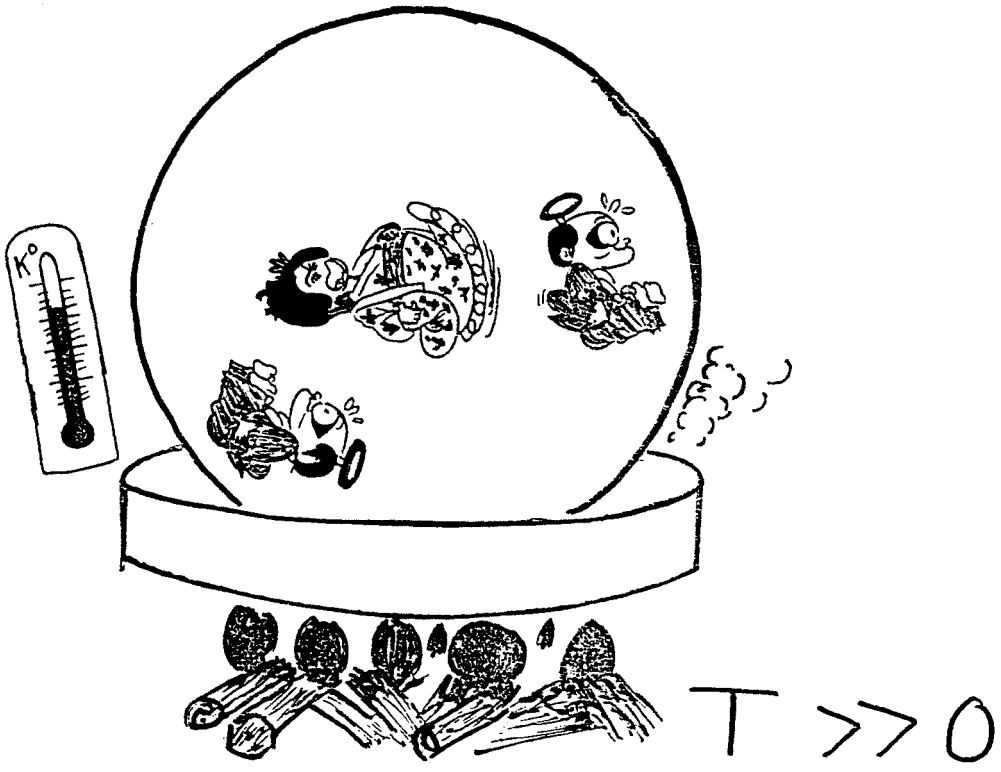


Fig. 21b

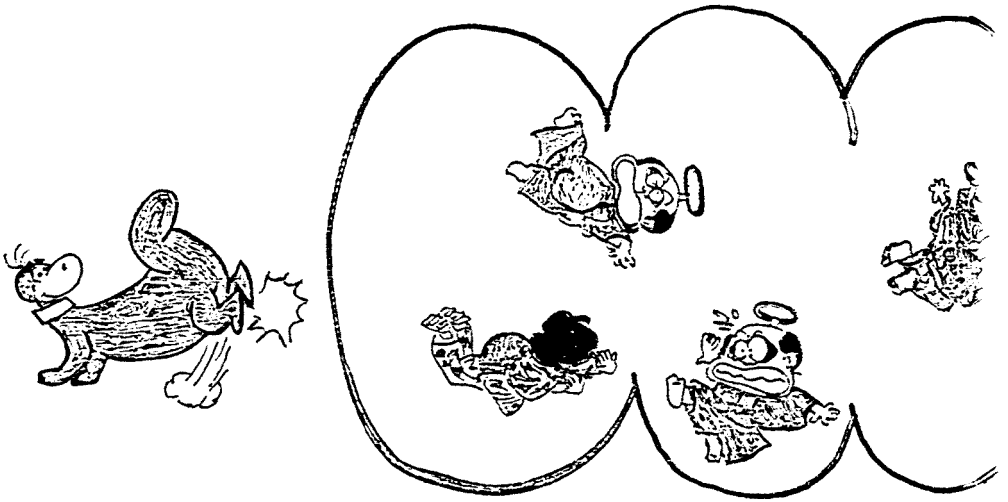


Fig. 21c

Fig. 21. Quarks and gluon in many phases

mean the existence of the limiting temperature; rather system may undergo a phase transition [2]. Kislinger and Morley calculated a gluon self-energy diagram shown in Fig. 22 at finite temperature and have found a gluon gets mass [3a].

$$M_{\text{Gluon}} \propto T. \tag{6.3}$$

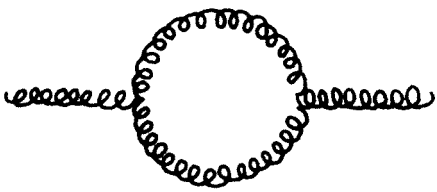


Fig. 22. The lowest order correction to a gluon propagator

Gluons become heavy and the long range force derived from them may be different from the confining force (Fig. 21b). Afer the detailed analysis of Freedman and McLerran, perturbative calculations have been steadily perfomed [3] though still there is a controversy over magnetic mass of gluons [3g–i].

Collins and Perry conjectured that at very high density hadrons overlap with each other and the quarks move freely inside the overlapped hadrons (Fig. 21c) [4].

MC studies of SU(2) Yang-Mills theory in the absence of dynamical quarks by McLerran and Svetitsky and by Kuti, Polonyi and Szlachanyi [5] have given the first numerical evidence for a second order transition from a confined phase to a deconfined one. Group at the University of Bielefeld and at the University of Illinois have performed MC simulations of the gluon matter at finite temperature in detail; for SU(3) Yang-

-Mills theory, they have observed first order phase transition at $T = 150$–200 MeV and ideal gas behavior of gluons at high temperature. It was observed that chiral symmetry breaking is restored around the transition temperature. See Ref. [2a] and [2h] of Part I and references therein.

Such studies of QCD in unusual environment are done not only for a theorist' fun and amusement. We hope that in high energy heavy ion collisions high temperature and density matter might be produced in a controlled experimental environment. To understand the data which might arise from such experiments, we may develop and study models of the quark-gluon system. MC simulation of lattice QCD probably provides the most fundamental information for such an analysis. For the study of hadronic matter, it is important to include quark loops in the calculation since they play a crucial role in screening; once we allow quark pair creation and annihilation, the long range force may be changed drastically. Theoretical conjectures were that the phase transition observed in the pure gauge calculation might be washed out by them [6]. In the presence of dynamical quark fields, the Polyakov line is no more a good order parameter for the confined and deconfined phases; Mathematically this is because the presence of quark fields breaks the symmetry under the center of the gauge group or physically because isolated heavy quarks can survive due to the quark pair creation.

7. *Thermodynamical quantities on a lattice*

We want to study thermodynamics of QCD. The essential ingredient is a partition function,

$$Z = \mathrm{Tr}\,(e^{-\beta(H-\mu N)}). \tag{7.1}$$

I apologize to the reader that I use the same notation β. Here β is $1/T$ *not* the coupling $2N/g^2$. We can rewrite the partition function as

$$Z = \int \mathscr{D}U \mathscr{D}\bar{\psi}\mathscr{D}\psi e^{-\int_0^\beta d\tau \int d^3x(\mathscr{L}+\mu n)} \tag{7.2}$$

with the periodic (anti-periodic) boundary condition for $U(\psi)$ in temporal direction. See Ref. [1b] for the proof of Eq. (7.2).

The parameters of a system are the temperature, T, and the chemical potential, μ. How are they introduced on a lattice? From Eq. (7.2) we see that size of our lattice in a temporal direction is just,

$$\beta = N_t a_t. \tag{7.3}$$

MC simulation of a finite temperature system is relatively easy: we can work on a smaller lattice.

It seems that chemical potential can be introduced by adding the following term to the action like a continuum case,

$$\mu\bar{\psi}\gamma_4\psi.$$

Hasenfratz and Karsch have found that chemical potential of this form makes energy density of free quarks diverge.

In the continuum the chemical potential appears in a Lagrangian as

$$\mathscr{L}_{\mathrm{F}} = \bar{\psi}[\partial_k\gamma_k+(\partial_4+\mu)\gamma_4+m]\psi. \tag{7.4}$$

Therefore a quark propagator is proportional to

$$\frac{1}{p^2+(p_4-i\mu)^2+m^2}. \tag{7.5}$$

On a lattice the action of free quarks in momentum space has the form,

$$S_{\mathrm{F}} = \int \mathscr{D}p\bar{\psi}_p\Delta(p)\psi_p,$$

$$\Delta(p) = \left(\frac{a}{2\pi}\right)^4\left[1-\kappa\sum_{\mu=1}^{4}\{(1-\gamma_\mu)e^{ip_\mu a}+(1+\gamma_\mu)e^{-ip_\mu a}\}\right]. \tag{7.6}$$

By replacing p_4 with $p_4-i\mu$, we get

$$\Delta(p) = \left(\frac{a}{2\pi}\right)^4\left[1-\kappa\sum_{l=1}^{3}\{(1-\gamma_l)e^{ip_l a}+(1+\gamma_l)e^{-ip_l a}\}\right.$$

$$\left.-\kappa e^{\mu a}(1-\gamma_4)e^{ip_4 a}-\kappa e^{-\mu a}(1+\gamma_4)e^{-ip_4 a}\right]. \tag{7.7}$$

Therefore we may introduce the chemical potential by changing the hopping parameter in a temporal direction to $\kappa\exp(+\mu)$ and $\kappa\exp(-\mu)$.

Energy densities, ε, and number density, n, is defined as

$$Z = e^{-\beta(\varepsilon-\mu n)V}, \quad V = (N_1 a_1)^3. \tag{7.8}$$

Then

$$\varepsilon = \frac{1}{V}\left(-\frac{\partial}{\partial\beta}+\frac{\mu}{\beta}\frac{\partial}{\partial\mu}\right)\log Z|_V,$$

$$n = \frac{1}{\beta V}\frac{\partial}{\partial\mu}\log Z|_V,$$

where

$$\frac{\partial}{\partial\beta} = \frac{1}{N_t}\frac{\partial}{\partial a_t}. \tag{7.9}$$

When we take the derivative of $\log Z$ regarding to any variable, we have two terms coming from S_{G} and S_{F},

$$(\log Z)' = \frac{1}{Z}\int \mathscr{D}U\mathscr{D}\bar{\psi}\mathscr{D}\psi(-S_{\mathrm{G}}'-S_{\mathrm{F}}')e^{-S}. \tag{7.10}$$

The first (second) term is considered to be the contribution from gluons (quarks).

8. Results of MC simulation with quark loops

I have run the simulation on a $2 * 8^3$ lattice with two flavors using the pseudo-fermion method. The gauge group SU(2) is replaced by its icosahedral subgroup. The hopping parameter is fixed to be 0.17 which would correspond to a very small quark mass in the quenched case. The number of gauge MC iterations is 100 including 20 thermalization except for $4/g^2 = 2.0, 2.2$ and $\mu = 0$ where it is 84. The number of pseudo-fermion iteration is 45 including 15 thermalization for each sweep of gauge fields.

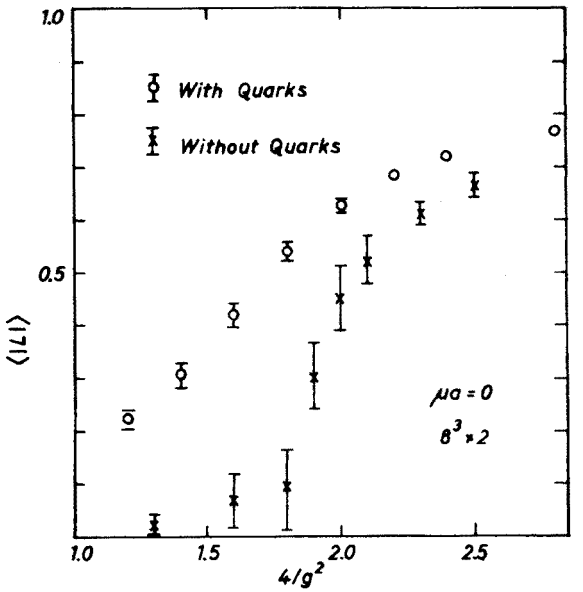


Fig. 23. Expectation value of the Polyakov line as a function of $4/g^2$ for zero chemical potential. The circles are the data obtained in the presence of quark loops. The crosses correspond to the pure gauge matter

In Fig. 23, I show the expectation value of the Polyakov line as a function of $4/g^2$ for $\mu = 0$. At high temperature (i.e. small g^2) the Polyakov line has large expectation value which implies the existence of isolated heavy quarks with only small supression due to finite temperature effects, while its value is small at low temperature. The characters of the system at high and low temperature are therefore different but heavy quarks are nevertheless deconfined in both phases. Its change is quite smooth, and no indication of a second order transition can be seen.

On the other hand, the gluon and quark densities, which are plotted in Figs. 24a and 24b, show rapid variation. Moreover the value of the quark energy density at high temperature is much larger than that of pure gluon system which agrees quite well with the "free gas" behavior at high temperature. Here "free gas" refers to the massless free bose or fermi fields on a lattice of the same size [7]. The energy density of gluons is as

large as 3/2 of the "free gas" (the dashed line in the figure). This suggests more degrees of freedom than those of simple ideal quark gluon gas. The system of quarks and gluons at these temperature regions looks rich in structure.

The rapid change in the energy densities occurs at the smaller value of $4/g^2$ than in the pure gauge case. This does not mean the transition temperature is lower than that of pure gauge theory because the lattice distance a at the same value of $4/g^2$ is different between two theories. As we see in Section 5, once we switch on the quark loops, the gauge configurations are pushed into more ordered state and the finite size effects become more

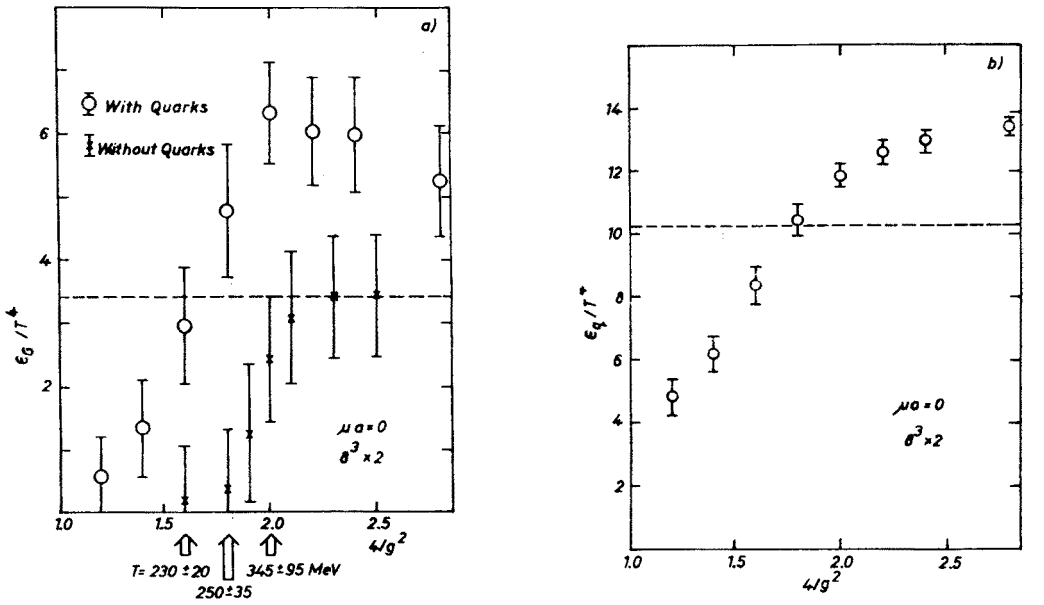


Fig. 24. Gluon energy density (a) and quark energy density (b) for zero chemical potential as a function of $4/g^2$. The dashed line gives the free field limit on the same lattice

serious. This may be interpreted as the shrinkage of the lattice distance drived by the quark loops.

In order to know the value of temperature in physical unit, we should evaluate the lattice distance a. Note that we cannot use the values in the literature which obtained without quark loops. I ran a simulation on a $N_t * N_x * N_y * N_z = 8 * 8 * 4 * 4$ lattice at $4/g^2 = 1.6$, 1.8 and 2.0 and measured Wilson loops on $t-x$ plane. The heavy quark potential is estimated by a Stack method. We fit the results to a Martin phenomenological potential [8] with the lattice distance and the constant part of the potential as parameters. The obtained temperatures are shown in Fig. 24a.

We can expect the rapid change of the quark gluon energy density between $T = 200$–350 MeV, which may be more drastic in case of SU(3).

Next we shall study the effects of the chemical potential. We plot the MC data in

Fig. 25–27 as a function of the chemical potential for $4/g^2 = 1.4$. As the chemical potential increases, the value of the Polyakov line increases very slowly and monotonically, while the thermodynamical quantities show peculiar behavior. At large chemical potential, isolated heavy quarks can survive longer than at the zero chemical potential. The gluon energy density shown in Fig. 26a increased quickly when we increase the chemical potential, i.e., the gluons are not independent of quark matter density and exhibit behavior far

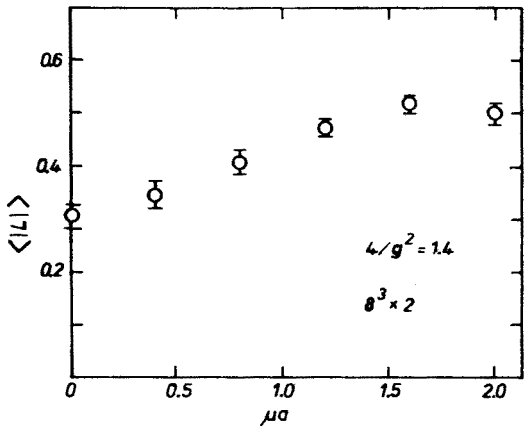


Fig. 25. Expectation value of the Polyakov line as a function of chemical potential for fixed temperature

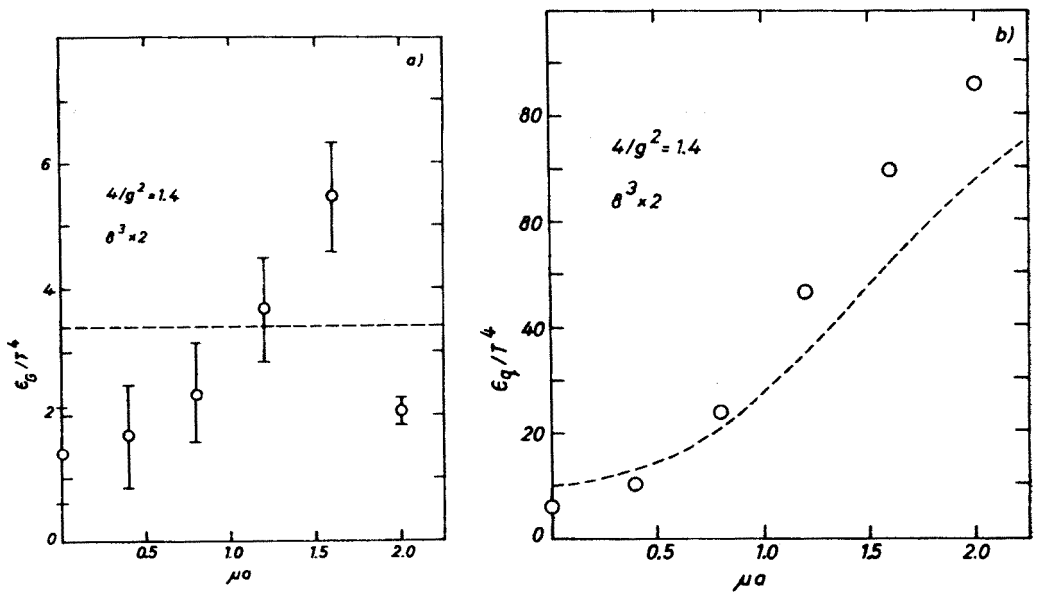


Fig. 26. Gluon energy density (a) and quark energy density (b) as a function of chemical potential for fixed temperature. The dashed line gives the free energy limit on the same lattice

from that of a "free gas". However it falls suddenly at large chemical potential. The quark energy density in Fig. 26b increases like a "free gas" but value is much higher. At these chemical potential regions, the free quark-gluon picture is not correct. There might be other degrees of freedom. The number density, n, shown in Fig. 27 also overshoots the "free gas" values at large chemical potential in a similar manner to quark energy density. To obtain the system with large chemical potential, higher density is required than that estimated from ideal gas equation.

In Table V, I compile the present situation of the simulations at finite temperature with quark loops.

This calculation was done at CERN, Frascati and Zaragoza. I am grateful to the theory divisions there for their hospitality. I wish to thank G. Parisi who has, with great

TABLE V

Compilation of MC experiments at finite temperature with quark loops. Here "phase transition" does not always mean phase transition in its mathematically exact sence, rather rapid change in thermodynamical quantities

Group	Color	Action	Method Lattice	Parameters	Observed Quantities "Phase Transition"
CERN[1]	SU(3)	Wilson	4th HOPE $8^3 * 2$	$6/g^2 = 4.9-5.1$ $\kappa = 0-0.05$	$\langle L \rangle$ No
Bielefeld I[2]	SU(3)	Wilson	4th HOPE $8^3 * 3$	$6/g^2 = 5.2-9$ $\kappa = 0.15, 0.20$	ε_G Yes
Cal Tech[3]	SU(3)	Susskind	Pseudo-Ferm $6^3 * 4$, $8^3 * 4$	$6/g^2 = 5.4-5.775$ $ma = 0.1, 0.2$	E_p, $\langle L \rangle$, ε_G Yes
Bielefeld II[4]	SU(3)	Susskind	Pseudo-Ferm $6^3 * 2$	$6/g^2 = 4.4-5.0$ $ma = 0.1$	$\langle L \rangle$, ε_G Yes
Illinois[5]	SU(3)	Susskind	Micro-cancl $8^3 * 4$	$6/g^2 = 4-7$ $ma = 0.08-0.10$	$\langle L \rangle$, ε_G, ε_q Yes
INS[6]	SU(2)	Wilson	Pseudo-Ferm $8^3 * 2$	$4/g^2 = 1.2-2.8$ $\kappa = 0.17$ $\mu a = 0-2.0$	$\langle L \rangle$, ε_G, ε_q Yes

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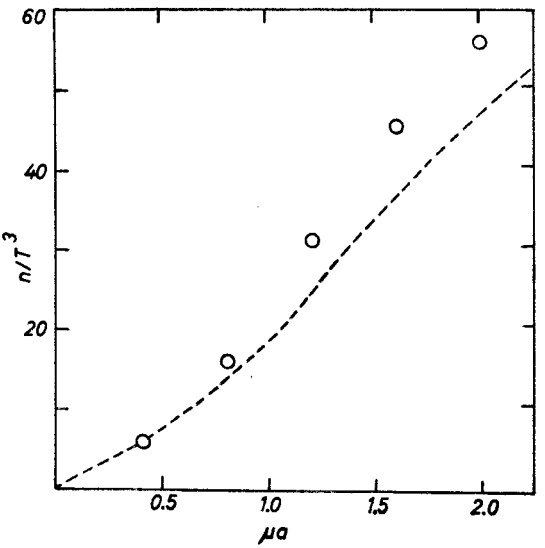

Fig. 27. Quark baryon number density as a function of chemical potential for fixed temperature. The dashed line gives the free energy limit on the same lattice

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