# FERMIONIC METHODS

# IN

# LATTICE GAUGE THEORY

Thesis

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## DECLARATION

Some of the work described in this thesis, notably the material in chapter 2 section 3 and chapter 4 section 3, was performed in collaboration with Drs. R.D.Kenway and A.Kenway. All other work in this thesis is entirely my own, except where otherwise indicated. Published work includes the following references


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## ABSTRACT

The inclusion of fermionic degrees of freedom into lattice gauge theories is examined. The doubling of fermion flavours on the lattice is reviewed and some of the methods for eliminating the unwanted species are presented. The connection between Susskind and Dirac-Kahler fermions is established and this leads to an explicit identification of the Susskind flavours in the lattice theory. It is shown how different masses may be given to the different flavours and the most local mass terms on the lattice are identified. The possibility of removing unwanted flavours by giving them a mass of order the lattice cutoff, and thus effectively decoupling them, is proposed. Methods for introducing dynamical fermions into lattice gauge theories are reviewed. The pseudo-fermion method is introduced and the Metropolis and two Langevin methods for implementing it are examined. The Schwinger model is reviewed and the pseudo-fermion methods are tested and compared both with one-another and with exact results for the massless continuum Schwinger model. The Langevin method is found to be the faster of the two methods, although more general considerations lead us to conclude that the Metropolis method will be more efficient in a simulation of QCD. In the case of two degenerate fermions the results are consistent with the known properties of the SU(2) Schwinger model. When one of the flavours is decoupled the measurements are in agreement with the one-species model. The prescription for removing the fermion degeneracy in which the square root of the fermionic determinant is used in the effective action for the gauge field fails.

CONTENTS

# CHAPTER 1

# INTRODUCTION

The language of gauge theory provides us with new and deep insights into the whole realm of high energy physics. The recent detection of the W and Z particles at CERN dramatically confirms our belief in the unified electro-weak interaction theory and the importance of gauge theories. We also have a gauge theory (QCD) for the strong interactions in which the hadrons behave as bound states of fundamental quark fields which interact via an octet of coloured gluons through the minimal Yang-Mills interaction. Moreover QCD exhibits the property of asymptotic freedom which allows us to obtain reliable calculations from perturbation theory of the short distance properties of the theory. These are in agreement with the scaling properties observed in deep inelastic scattering experiments.

However, the large distance behaviour remains an unsolved problem due to infrared singularities. As we look at lower momentum scales the strength of the QCD coupling constant moves out of the perturbative regime and it becomes more difficult to disentangle non-perturbative effects from those that are genuinely perturbative in experiments. Moreover the fact that up until now we have only observed uncoloured bound states leads one to suspect the possibility that long range forces might permanently confine quarks and gluons within physical hadrons. In order to reconcile the apparently contradictory aspects of infrared slavery and asymptotic freedom and to understand quark confinement it appears necessary to study the

field theory beyond the framework of perturbation theory.

Lattice gauge theory is such a non-perturbative technique in which space, or space-time, is discretized by introducing an underlying lattice. In this way it is possible to use the similarity with statistical mechanics inherent in the functional integral formalism to investigate the theory. It is clear that the lattice will destroy the Lorentz invariance of the theory which will only be restored in the continuum limit. However the gauge invariance, which is the central feature of the theory, remains explicit on the lattice. The lattice description enables us to study the theory either through strong coupling expansions of the sort used in statistical mechanics or to carry out direct numerical simulations, such as the widely used Monte Carlo algorithm.

In this introduction we will firstly examine the formulation of the theory, as originally proposed by Wilson (1974), and its connection with the continuum Yang-Mills theory (Yang and Mills 1954). Mention will be made of the strong coupling expansion and some of the similarities with statistical mechanics. The Wilson loop will be introduced and the property of confinement, and how it arises naturally in the strong coupling regime, will be examined. The renormalization group structure will then be discussed and the appearance of a mass scale through dimensional transmutation illustrated. The use of Monte Carlo methods to study the theory will be explained and the part that phase transitions play will be discussed. Measurements of the string tension will be discussed, as will the recent attempts at measuring the hadron and glueball spectrums.

There are a number of ways of introducing a lattice, the most

widely used of which is the Euclidean lattice. The connection is made with Minkowski space through a Wick rotation which enables us to reinterpret our results in the usual physical space at the end of any calculation. For example, the evolution in Minkowski space according to the operator exp(-iHt) is replaced under a Wick rotation by exp(-Ht) and no information is lost in the process. Indeed, it is just such an identification between the two spaces that is used in the hadron and glueball mass calculations, as we shall see. It is usual to introduce a hypercubical lattice of spacing a in this Euclidean space of d dimensions. This choice is not dictated by the theory in any way, except in so far as it appears to be the simplest choice and its remarkably simple geometric properties make it very convenient in actual calculations. However any lattice is in principle possible and there has been some interest of late in formulations on very different types of lattices. The only restriction is that the correct continuum limit be obtained in the limit that the lattice spacing vanishes. Christ, Friedberg and Lee (1982) have examined a formulation of lattice gauge theory in which the lattice sites themselves are chosen randomly. The question of different lattice formulations is intimately connected with the renormalization group and the role of fixed points, which we shall touch upon later.

The field theory is quantized using the path integral formulation in which we define an action $S[\phi]$ depending upon classical fields that we denote collectively by $\phi(x)$. Physical quantities are then defined in a manner familiar in statistical physics by

$$\langle F(\phi)\rangle = \frac{\int \mathcal{D}\phi\, F(\phi) \exp(-S(\phi))}{\int \mathcal{D}\phi \exp(-S(\phi))} \tag{1.1}$$

where the denominator is the partition function of the theory. In the lattice theory we do not encounter the usual problems associated with this formula in field theory, where we must choose precisely the functional space of classical fields and the integration procedure (unless we limit ourselves to perturbation theory given in terms of Gaussian integrals). On a finite lattice (i.e. with a space-time volume cutoff) the functional integral is well defined as the simple product (now finite or, on an infinite lattice, denumerable) of the integrals over the field values at every site of the lattice. There is an alternative approach in which space-time remains Minkowskian and only the spatial dimensions are discretized. In this Hamiltonian formulation the fields may be quantized following the usual canonical prescription, however this method will not be pursued here.

The equivalence between the Euclidean lattice formulation and its statistical counterpart is central to our understanding of the theory. Indeed the continuum field theory may be recovered from the statistical mechanics model when the correlation length of the lattice theory diverges and the underlying lattice is no longer important. Then the path integral corresponds to a sum over all configurations and the action is related to the energy of a configuration. An external source in the Euclidean field theory corresponds to a magnetic field (in the context of, for example, the Ising or Heisenberg models of ferromagnetism) and a classical field to the magnetization. The propagator of the field theory is the correlation function of the spin system and the mass gap corresponds

to the inverse correlation length. Moreover we can study the theory in both perturbation theory and strong coupling in just the same way as it is possible to make low and high temperature expansions in statistical mechanics.

In constructing a lattice gauge theory we wish to keep the gauge symmetry explicitly in the lattice formulation and recover the Yang-Mills theory in the continuum limit. An alternative approach in which we simply discretize the continuum theory does not exhibit the gauge symmetry on the lattice, although it will be restored in the continuum limit. The first theory to have a local gauge symmetry on a lattice was the Ising lattice gauge theory of Wegner (1971). His interest in introducing a local invariance group arose from the fact that magnetization is forbidden in such a theory. However, despite the absence of a local order parameter he showed that this model had a phase transition, and he suggested how the various phases could be labelled and distinguished. Wilson (1974) generalized the Ising lattice gauge theory to continuous gauge groups, and it is this formulation that we will discuss here.

The basic building blocks for a lattice gauge theory are the variables that live on the links of the lattice. In the case of an SU(N) lattice gauge theory the link variables are SU(N) group matrices $U_\mu(\underline{n})=\exp[iB_\mu(\underline{n})]$, where $\mu$ labels the direction of the link (i.e. $\mu=1,2,3,4$), $\underline{n}$ labels the sites of the lattice, $B_\mu(\underline{n})=\frac{1}{2}agT_iA^i_\mu(n)=\frac{1}{2}agT.A_\mu(n)$ and the $T_i$ are the generators of SU(N). The Greek indices that are used to label the lattice directions are not to be regarded as Lorentz indices since they are used only as a matter of notational convention and no attempt is made to match indices in equations. Since the group volumes are finite the

integrals that we encountered in the path integral formulation eq.(1.1) are well defined. Local gauge invariance can be stated very elegantly on the lattice by imagining a colour frame of reference at each site. By putting an SU(N) matrix G(n) at every site of the lattice it is possible to make the orientation of the colour space locally arbitrary. Under a gauge transformation the link variables transform as

$$U_\mu(n) \longrightarrow G(n)\, U_\mu(n)\, G^{-1}(n+\hat{\mu}) \tag{1.2}$$

which we recognize as the simplest local generalization of a global SU(N) invariance. To construct an action that incorporates this local symmetry it is clear that we require objects that are built out of the products of U matrices around closed paths. These quantities are locally gauge invariant because the SU(N) colour indices are then all contracted locally. The most local contours are the elementary squares of the lattice, called plaquettes, and the resulting action is (Wilson 1974)

$$S(U) = \beta \sum_{n,\mu\nu} \left\{ 1 - \frac{1}{N} Re\, tr\, U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu^{+}(n+\hat{\nu}) U_\nu^{+}(n) \right\} \tag{1.3}$$

where links in the backward directions are given by $U_{-\mu}(n+\hat{\mu}) = U_\mu^{-1}(n)$ and $\beta$ is related to the coupling g by $\beta = 1/2g^2$.

It is now necessary to check that this action reduces to the ordinary Yang-Mills action in the continuum limit. To do this we make the long-wavelength approximation and Taylor expand the slowly varying field $B_\mu(n)$;

$$B_\nu(n+\hat{\mu}) = B_\nu(n) + a\,\partial_\mu B_\nu(n) + O(a^2) \tag{1.4}$$

The action (1.3) may then be rewritten using the Baker-Campbell-Hausdorff identity

$$\exp(ax)\exp(ay) = \exp\Big(ax + ay + \frac{a^2}{2}[x,y] + \frac{a^3}{12}\big([x,[x,y]] - [y,[x,y]]\big) + O(a^4)\Big) \tag{1.5}$$

Consequently

$$UUU^\dagger U^\dagger = \exp\left\{ia^2 g\left(\partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]\right) + O(a^3)\right\} \tag{1.6}$$

where we have dropped the indices on the U matrices. The leading term here is clearly the conventional Yang-Mills field strength $F_{\mu\nu}$ with corrections in the exponent of higher order in $a^2$ which will not contribute in the classical continuum limit. For smooth classical fields that vary only over distance scales large compared with the lattice spacing a we have $a^2 g F_{\mu\nu} \ll 1$ and the exponential in the action can be expanded as

$$\begin{aligned} \mathrm{tr}\, UUU^\dagger U^\dagger &\simeq \mathrm{tr}\, \exp(ia^2 g F_{\mu\nu}) \\ &= \mathrm{tr}\, 1 - \tfrac{1}{2} a^4 g^2\, \mathrm{tr}\, F_{\mu\nu}^2 + O(a^6) \end{aligned} \tag{1.7}$$

where $\mathrm{tr} F_{\mu\nu} = 0$ since the trace of the generators vanishes and the tr1 term has no dynamics and can thus be dropped. Finally the replacement

$$\sum_{n,\mu\nu} \longrightarrow \int \frac{d^4x}{a^4} \sum_{\mu\nu} \tag{1.8}$$

establishes the equivalence with the usual Euclidean Yang-Mills action:

$$S_{Yang\text{-}Mills} = \frac{1}{4} \int d^4x \, (F^i_{\mu\nu})^2 \tag{1.9}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu]$ and $A_\mu = A^i_\mu T^i$. It is the local invariance that we have built into the lattice action that ensures that we recover the standard field strength tensor $F^i_{\mu\nu}$ of the Yang-Mills theory. Moreover the resulting theory is clearly Euclidean O(4) invariant and the discrete cubic invariance of the original action has disappeared into the irrelevant terms of higher order in the lattice spacing a. Actions that differ from the Wilson action by such irrelevant terms will clearly have the same continuum limit and are being studied (Symanzik 1982; Martinelli, Parisi and Petronzio 1982; Weisz 1982; Berg, Meyer, Montvay, and Symanzik 1983) as a means of calculating "closer" to the continuum limit.

In order to see how confinement arises naturally in the strong coupling regime of the theory we consider a Wilson loop W(C) which consists of a product of the U matrices around a closed contour C of links. However it is instructive to firstly consider the corresponding object in the continuum theory, which is the loop correlation function:

$$\langle tr\, P \exp\left(ig \oint A^i_\mu T^i dx^\mu\right) \rangle \tag{1.10}$$

where P denotes the path ordered product. This is simply related to the heavy quark potential V(R) by observing that we have introduced an external current $J^i_\mu$ describing a closed current loop (i.e. $J_\mu$=1 on the contour C and vanishes elsewhere). Consequently the expectation value (1.10) of the loop integral may be interpreted as the ratio of the partition function for the system which includes the external charges Z(J) to that in which they are omitted Z(0), and this can be related to the free energy F(J) of the system with the charges:

$$\begin{aligned} \langle \mathrm{tr}\, P\exp(ig\oint A_\mu dx^\mu)\rangle &= Z(J)/Z(0) \\ &= \exp\left[-(F(J)-F(0))\right] \end{aligned} \tag{1.11}$$

If we consider a contour of length T in the time direction and R in the spatial directions then what we are measuring is the matrix element of the evolution operator exp(-HT) between initial and final states that consist of an infinitely heavy $q\bar{q}$ pair a distance R apart (H is the Hamiltonian of the gauge theory). This is then just the difference between the ground state of the Hamiltonian with the charges included and with them omitted. Since the charges are static the energy difference is completely potential. Thus

$$V(R) = -\lim_{T\to\infty} \frac{1}{T} \ln \langle \mathrm{tr}\, P\exp(ig\oint A_\mu dx^\mu)\rangle \tag{1.12}$$

so that if V(R) increases as $|R|$ at large distances then an infinite amount of energy would be required to separate the quarks, and they are consequently confined. On the other hand if V(R) is independent of R then the charges could easily be pulled free. It is possible to show that in the U(1) gauge theory we recover Coulombs law for weak

coupling $g^2 << 1$.

In the context of lattice gauge theory this loop correlation function (1.10) was precisely that introduced by Wegner (1971) to serve as an order parameter. This is possible since the high and low temperature phases of the gauge-spin models may be identified with exponential area and perimeter law behaviour respectively of the loop correlation function W(C). In order to establish the relationship between W(C) and confinement in the lattice model we require the following properties of the Haar measure:

$$\int \mathcal{D}U = 1 \,, \quad \int \mathcal{D}U\, U_{ij} = 0 \,, \quad \int \mathcal{D}U\, U_{ij} U^{\dagger}_{kl} = c\, \delta_{il}\, \delta_{jk} \qquad (1.13)$$

where c is a normalization constant. The leading behaviour of $\langle W(C) \rangle = \langle \prod_C U_\mu(\underline{n}) \rangle$ is obtained by expanding the exponential and considering only the first non-trivial term. The lowest order term is obtained by diagrammatically covering the interior of the contour C with plaquettes. Since each plaquette is associated with a factor of $1/g^2$ this procedure of minimally tiling the contour C gives the leading order term:

$$\left\langle \prod_C U_\mu(n) \right\rangle = \left(\frac{1}{g^2}\right)^{N_c} = \exp\left(-\ln g^2 \times \frac{\text{Area}}{a^2}\right) \qquad (1.14)$$

where $N_C$ is the minimal number of plaquettes contained in C and is a measure of the area. As we saw in eq.(1.12) this leads directly to a linear confining potential for heavy quarks, and the leading term in the dimensionless string tension K at strong coupling is the coefficient $\ln(g^2)$. Thus confinement arises naturally in the strong coupling regime of the lattice gauge theory.

We now look at some of the renormalization group properties of the theory and particularly at the appearance of the $\Lambda$ parameter, which is the natural mass scale of the theory. In the action (1.3) the only parameter is the dimensionless coupling g, and the lattice spacing a appears implicitly. On purely dimensional grounds it is possible to establish the relationship between any mass m in the theory and the lattice regularization

$$m = \frac{1}{a} f(g) \tag{1.15}$$

In the continuum limit the cutoff must be much larger than the physical masses, i.e. the correlation length must be much larger than the lattice spacing and in the limit $a \to 0$ will extend over an infinite number of lattice sites. In the language of statistical physics this means that the system should approach a continuous phase transition point (Wilson and Kogut 1974). Because we are interested in the continuum system it is important to approach the $a \to 0$ limit carefully by readjusting the coupling constant (i.e. renormalization). The physical quantities of the theory, such as correlation lengths, must be kept finite as the lattice spacing vanishes and this will determine how the coupling constant consequently changes. This is why the understanding of the phase structure and critical points is so central to lattice gauge theories. It is clear from eq.(1.15) that it is only possible to define a non-trivial continuum limit if there exists a critical coupling $g_{crit}$ such that $f(g) \to 0$ as $g \to g_{crit}$. The continuum limit of the lattice SU(2) and SU(3) models are found as $g \to 0$, and $g^* = 0$ is the infrared unstable fixed point of the theory in the neighbourhood

of which we can use perturbation theory (Gross and Wilczek 1973,1973). In the continuum limit all physical quantities should become independent of the lattice cutoff (i.e. they should be renormalization group invariant):

$$a \frac{d}{da} m = 0 \qquad (a \to 0) \tag{1.16}$$

The beta function, which gives the relationship between the coupling g and the lattice spacing a, is defined by

$$\beta(g) \equiv -a \frac{d}{da} g = -\beta_0 g^3 - \beta_1 g^5 - \ldots \tag{1.17}$$

where the coefficients $\beta_0$ and $\beta_1$ may be calculated in perturbation theory and are found for SU(N) gauge theory to be (Gross and Wilczek 1973; Politzer 1973; Caswell 1974; Jones 1974):

$$\beta_0 = \frac{11}{3}\left(\frac{N}{16\pi^2}\right) \quad , \quad \beta_1 = \frac{34}{3}\left(\frac{N}{16\pi^2}\right)^2 \tag{1.18}$$

From the beta function we observe that the theory is asymptotically free, i.e. at very short distance scales the coupling vanishes and the theory behaves as if it were free. Expressing m in terms of eq.(1.15) the condition (1.16) becomes

$$f(g) + \beta(g) \frac{df(g)}{dg} = 0 \tag{1.19}$$

This equation may be solved for f(g), and using eq.(1.17) we obtain the well known $\Lambda^{latt}$ parameter which is the renormalization group invariant mass scale of the theory:

$$\Lambda^{latt} = \frac{1}{a} \exp\left(-\int^{g} \frac{dg'}{\beta(g')}\right) \qquad (1.20)$$
$$= \frac{1}{a} \exp(-1/2\beta_1 g^2)(\beta_0 g^2)^{-\beta_1/2\beta_0^2}[1 + O(g^2)]$$

All the masses in the theory can then be expressed in terms of $\Lambda^{latt}$ and ratios of dynamically generated masses must be pure numbers that depend only on the gauge group. Thus, once the mass scale is set all the masses of the theory are determined with no free parameters. Also it is clear from the form of eq.(1.20) that $\Lambda^{latt}$ does not have a perturbative expansion and the mass generation is consequently a non-perturbative effect. The regime in which (1.20) holds is known as the scaling region of the theory. In order to compare the lattice calculations with those done in the continuum theory it is necessary to relate $\Lambda^{latt}$ to the various $\Lambda$-parameters of the continuum regularization schemes. This may be done by calculating both the divergent and finite parts of the one-loop coupling constant renormalization in the way that is usually used to relate different continuum renormalization schemes. This calculation has been done by Hasenfratz and Hasenfratz (1980) giving

$$\Lambda^{mom}_{a=1} = 57.5\,\Lambda^{latt} \quad \text{for } SU(3)$$
$$= 83.5\,\Lambda^{latt} \quad \text{for } SU(2) \qquad (1.21)$$

for the pure gauge theory (i.e. without fermions).

Having established that QCD is an asymptotically free theory and that the lattice theory confines quarks at strong coupling the question becomes one of whether or not there is a phase transition in the intermediate region. It is known that such a transition occurs

in the U(1) gauge theory and there is a critical point separating the charge confining phase from the free charge phase. Indeed, the introduction of the loop correlation function by Wegner (1971) was in order to distinguish between the two phases of the theory. There are a number of different methods for mapping out phase diagrams which have been used in statistical mechanics with varying degrees of reliability. High- and low-temperature expansions, duality transformations, spin-wave analyses and mean field theory have all proved quite useful. In actual simulations of gauge theories the most frequently used technique is that of looking for a hysteresis loop in a thermal cycle. We choose some cross-section of the phase space and adiabatically move the system forward and backwards along this path, typically by varying some parameter "$\beta$". At each "temperature" step a number of iterations are performed and the system approaches some sort of equilibrium. However, if there is a phase transition, with a critical point $\beta_c$, then in the neighbourhood of $\beta_c$ the system does not really reach equilibrium because of the increase in the relaxation time and there will be a mis-match on the return cycle when we measure physical quantities. An alternative method is to do a mixed phase run in which the initial state of the system is divided into two halves, one of which is ordered and the other disordered. It is possible to tell if there is a phase transition by observing how the system evolves from this "mixed-phase" configuration. The phase diagrams of a number of different lattice models have been extensively investigated and the numerical results seem to indicate that a phase transition which would separate the free and the confining regions, such as that observed in the U(1) theory, does not occur in four dimensional SU(2)

or SU(3) gauge theories and that the strong coupling phase persists to the limit of vanishing bare coupling.

Before proceeding to discuss some of the calculations and results obtained in lattice gauge theory we shall firstly give an outline of how the Monte Carlo procedure operates (see, for example, Binder 1976). A measurement of some physical quantity $f(\phi)$ is formally done by evaluating the functional integral eq.(1.1). However, it is clear that even for discrete gauge groups on small lattices it is not possible to generate all configurations in any reasonable computer time. The Monte Carlo algorithm provides an approximate scheme for evaluating the functional integral by generating a sequence of configurations that mock the equilibrium behaviour of the system. Starting from some gauge configuration $\{U\}$ (which is usually taken to be either random or completely ordered) the Monte Carlo algorithm will generate a new trial configuration $\{\tilde{U}\}$ according to a definite transition probability $P(U\rightarrow\tilde{U})$. There is considerable freedom of choice in this probability distribution since detailed balance only requires that

$$e^{-S(U)}P(U\rightarrow\tilde{U}) = e^{-S(\tilde{U})}P(\tilde{U}\rightarrow U) \qquad (1.22)$$

which ensures that the master equation has a solution which is the desired equilibrium probability distribution. More general constraints on stochastic processes obviously require that $P(U\rightarrow\tilde{U})\geq 0$ and $\sum_{U} P(U\rightarrow\tilde{U})=1$.

We generate a sequence of configurations $\{U^i\}$ (a Markov chain) according to the Boltzmann distribution. Starting from $\{U\}=\{U^i\}$ a new trial configuration $\{\tilde{U}\}$ is determined, which usually differs from

$\{U\}$ in only one dynamical variable. In the Metropolis method (Metropolis et al. 1953) we calculate the change in the action between the two configurations

$$\Delta S = S(\tilde{U}) - S(U) \tag{1.23}$$

If $\Delta S$ is negative (i.e. the new configuration lowers the action of the system) then the change $\{U\} \to \{\tilde{U}\}$ is always accepted and $\{U\}$ is updated. On the other hand if $\Delta S$ is positive we accept $\{U\}$ with probability given by the Boltzmann factor $\exp(-\Delta S)$: if $\exp(-\Delta S) > R$ then the new configuration is accepted and otherwise it remains unchanged, where R is a (pseudo-) random number with uniform probability distribution over the unit interval. If in this case ($\Delta S > 0$) we were to reject $\{U\}$ outright the action would decrease monotonically and we would eventually attain a classical solution corresponding to a minimum of the action (and if there were more than one minimum it would be possible for the system to get trapped into a metastable state of artificially high action). However, by comparing in this way with the Boltzmann factor we correctly take care of the quantum fluctuations. This algorithm guarantees that the sequence of configurations that we generate eventually reaches a regime of statistical equilibrium where the probability of any particular configuration occurring is given by the Boltzmann distribution $\exp(-S(U))$. It then follows that

$$\langle F(U) \rangle = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} F(U^{(i)}) \tag{1.24}$$

This equality holds independently of the particular choice of

$P(U \rightarrow \tilde{U})$, although inappropriate choices may lead to very slow convergence.

An alternative to the Metropolis method that is very efficient in some situations is the heat bath method (Creutz 1980; Rebbi 1980). If we were to consider repeating the Metropolis procedure many times on a given link it would eventually generate a new link variable with the Boltzmann probability (this is sometimes referred to as the modified Metropolis method). This procedure is equivalent to choosing the new link variable $U'_{ij}$ from amongst all its possible values with a probability distribution proportional to $\exp(-S(U'_{ij}))$ with all the other U's being kept fixed. Although the method is generally harder to implement in practice, it will usually converge significantly faster and there will be fewer problems with temporal correlations since the new link variable is not related to the old one, as it is in the Metropolis algorithm. The SU(2) heat bath takes advantage of the simplicity of the Pauli algebra and is quite fast. An SU(3) algorithm which uses SU(2) subgroups of SU(3) (Cabibbo and Marinari 1982) seems to be superior to the standard Metropolis algorithm for SU(3) (Bowler and Pendleton 1983).

Although the general principles involved in a Monte Carlo simulation can be precisely formulated there is in practice a good deal of freedom in their application. This freedom can, in any particular calculation, be usefully exploited depending upon the particular measurements and objectives, in much the same way as in an experiment. We will only mention some of the more important of these considerations here. The locality of the action (i.e. that it only explicitly couples neighbouring dynamical variables) is clearly very important in implementing a simulation. Non-localities can arise as

a result of partial summations over some of the variables in the construction of an effective action, as we shall see later when fermions are introduced into the dynamics.

The actual size of the lattice used should, of course, be sufficiently large to accommodate the relevant mass scales of the theory without introducing unmanageable finite size effects. Ideally, if $\xi$ is some physical length scale of the theory (eg. the correlation length) then we would choose $a \ll \xi \ll L$, where a is the lattice spacing and L is the total physical size of the lattice in any direction. In practice we are limited in the size of lattices by the computing power available, and a careful understanding of the various necessary approximations is essential. Such considerations form a separate study in themselves and we shall only touch upon the most important points here. Finite size scaling theory can often enable us to relax the condition $\xi \ll L$ (Hamer and Barber 1980) and modifications of the lattice action (Symanzik 1982) can also enable the condition $a \ll \xi$ to be relaxed by more closely fitting the continuum action. Bulk quantities, such as the internal energy, can often be measured on fairly small lattices whereas values of more widely separated observables, such as Wilson loops and correlation functions, are more difficult. Such non-local observables suffer from both the finite size of the lattice and the fact that the quantity being measured is often small and results from large cancellations, with the resultant large statistical fluctuations. It is often necessary to weigh the advantages of a larger lattice against the larger number of Monte Carlo updates that can be performed on a smaller lattice with the same computer resources.

The boundary conditions of a finite system are also important,

particularly in higher dimensions where the boundary contains a significant proportion of the lattice sites (eg. on an $8^4$ lattice there are more than twice as many sites on the surface as in the interior). Periodic boundary conditions on the gauge variables are almost universally used, but other more complicated boundary conditions have been considered in various contexts. In particular, twisted boundary conditions (t'Hooft 1979), or other variations in which periodicity is enforced modulo some transformation of the edge links, can be used and have the effect of introducing topological excitations into the system. It can sometimes also be important to consider the initial configuration from which a simulation is run. Since it is only configurations obtained after equilibrium has been reached that are usually of interest it is desirable to reduce the transient time that it takes for the system to reach equilibrium. Starting from different initial configurations can serve as a check that equilibrium has been reached, since the results should be independent of the particular initial configuration.

The recent interest in simulating lattice gauge theories lies in its application to QCD, because ordinary perturbative analysis does not extend into the strong coupling region which seems to determine much of the physics of the theory. We will briefly discuss here some of the quantities that have been measured in lattice QCD, although the reader is referred to some of the recent reviews of the subject for further details (see, for example, Kogut 1979 and 1983; Creutz, Jacobs and Rebbi 1983). The string tension, which measures the large distance attractive force felt by two static quarks, is obtained from measurements of the Wilson loop using the identity eq.(1.12). In order to factor out the perimeter dependence, which arises from the

self energy of the heavy quarks, it is usual to consider rectangular Wilson loops W(I,J), of width I and J in two directions. The quantity (Creutz 1980)

$$\chi(I,J) = -\ln\left(\frac{W(I,J)W(I-1,J-1)}{W(I,J-1)W(I-1,J)}\right) \tag{1.25}$$

is then a measure of the string tension for appropriately large values of I and J (in practice these values are quite limited). The results, initially obtained by Creutz (1980) and subsequently reproduced by a number of people, give agreement in the strong coupling regime with the strong coupling prediction and then behave in a manner consistent with scaling before tailing off into the perturbative regime. From the envelope of the curves, obtained from different sizes of Wilson loops, the string tension K(g) with the expected scaling behaviour may be extracted

$$\begin{aligned} K(g) &= \sigma a^2(g) \\ &\simeq \frac{\sigma}{\Lambda^2}\left(\beta_0 g^2\right)^{\beta_1/2\beta_0^2} \exp\left(1/2\beta_0 g^2\right) \end{aligned} \tag{1.26}$$

and the latest measurements (Creutz and Moriarty 1982) indicate $\sigma = (2.8 \pm 0.9) \times 10^4 \Lambda^2$ for SU(3). This measurement does not really determine the string tension, but rather by assuming the string tension to be a basic observable, it sets the value of $\Lambda^{latt}$ and thus determines the scale for all the physical quantities of the theory without any further adjustable parameters.

Since QCD is a confining theory we do not expect there to be long range interactions in the theory and hence there will be no massless mediating particles. Consequently the mass spectrum should begin

with some non-zero mass state which is identified with the mass $m_g$ of the lowest lying glueball state, also called the mass gap. In the absence of quarks this lowest glueball must be stable, although the coupling to quarks could mean that the state becomes broadened. There has been considerable effort to calculate $m_g$ using Monte Carlo techniques (Ishikawa, Teper and Schierholz 1982; Berg and Billoire 1982a,b; Michael and Teesdale 1982) and there is now broad agreement on the lightest glueball mass of $m_g = 750 \pm 50$ MeV (using $\Lambda_{mom} = 200$ MeV), which appears to scale properly. The measurements are carried out by choosing some appropriate plaquette operator $O(\underline{x},t)$ and considering the connected correlation function

$$G_c(\underline{x},t) = \langle O(\underline{x},t)\, O(\underline{0},t) \rangle \qquad (1.27)$$

By inserting a complete set of energy-momentum eigenstates and summing over $\underline{x}$, which picks out the zero momentum state, we see that

$$G_c(t) \equiv \sum_{\underline{x}} G_c(\underline{x},t) \propto e^{-m_g t} \qquad (1.28)$$

and the mass may be measured from the exponential fall-off of the propagator. The measurements are complicated by the fact that higher states will in general also couple to the operator $O(\underline{x},t)$ and they consequently contribute to $G_c(t)$. Moreover, it turns out that the correlation length $(1/m_g)$ is rather small over the region of coupling where Monte Carlo is possible and consequently the propagator falls off rapidly and becomes of the same order as the statistical fluctuations after only 3 or 4 lattice spacings. A variety of techniques have been developed to handle these difficulties, mainly

involving suitable choices of the operator $O(\underline{x},t)$ which minimize the mixing with higher excitations. Similarly it is possible to measure higher mass states by projecting out the relevant operators, although this is more difficult and the measurements are subject to larger statistical errors.

A number of other interesting and important calculations have been made in lattice QCD, such as the restoration of rotational invariance in the scaling regime, and various other physical quantities have been studied, including the deconfining temperature and the quark potential. However we shall confine ourselves here to a discussion of the prospect of calculating the hadron spectrum of QCD which has emerged recently (Hamber and Parisi 1981; Weingarten 1982; Marinari, Parisi and Rebbi 1981; Hamber et al. 1982; Bernard, Draper and Olynyk 1982; Bowler et al. 1982) In order to calculate particle masses a set of gauge field configurations is generated using the usual Wilson action. For each gauge field configuration the quark propagator $G(n,0)$ is calculated, from which the various particle propagators are constructed. By summing over the spatial directions the particle masses may be extracted from the large time behaviour. For example, the pion state is given by $\bar{\psi}(n)\,\gamma_5\,\psi(n)$ and the time-slice propagator is

$$\sum_{\underline{n}} \langle \pi(n)\,\pi(0)\rangle = \sum_{\underline{n}} \sum_{q} \frac{\exp(iq.n)}{q^2 + m_\pi^2} = \sum_{q_4} \frac{\exp(iq_4 n_4)}{q_4^2 + m_\pi^2} \sim e^{-m_\pi n_4} \tag{1.29}$$

Without going into any detail on these calculations a few essential features nevertheless emerge. Although the calculations are subject to an array of problems that stem from finite size and statistical

effects, many of the crucial features of QCD are seen. The pion appears as the lightest meson, and can thus be interpreted as a Goldstone boson by a suitable extrapolation to vanishing mass. The fermionic condensate $\langle\bar{\psi}\psi\rangle$ has been measured, and the rho is measured to be heavier than the pion, with a mass that remains finite in the limit of vanishing pion mass, provided that $m_\pi^2 \propto m_q$ is used to define $m_{crit}$. It has become clear that there are many features of the finite lattice approximation that have an important effect upon the measurements which need to be more thoroughly understood before reliable mass calculations can be done. The necessarily small lattices on which the simulations are run present immediate problems when we consider the physical size of the lattice, which in most cases is approximately that of a proton. Moreover there are finite temperature effects associated with the finite size of the lattice. Recently a discrepancy has emerged between the mass scales given by the string tension and the rho mass which needs to be understood. The correlations between successive gauge configurations presents problems in obtaining truly independent statistical data and the number of configurations over which measurements are averaged is rather small. The algorithms for finding the quark propagators are slow in the region of small quark masses and as a result all measurements are made for quark masses greater than approximately 200MeV and it is necessary to extrapolate to light masses, thus introducing more uncertainties into the analysis.

Thus, having established the principle features of lattice gauge theory and illustrated some of its successes we now move on to the question of incorporating fermions into these theories. This is by no means straightforward and, while it is true to say that very

significant steps have been made in understanding and overcoming some of the problems, much remains to be done. While the major part of the work to date has been in the context of one- and two-dimensional models, our foremost goal remains that of understanding QCD, and the usefulness of the various models and approximations encountered is always essentially measured in relation to their application to QCD.

In chapter 2 we examine the problem of transcribing the Dirac equation onto the lattice. It is well known that the most straightforward description leads to the "doubling" problem in which the continuum limit of the theory contains many more fermion flavours than we would like. A number of proposals for overcoming or reducing this flavour degeneracy are discussed. Wilsons method explicitly breaks chiral symmetry and the SLAC method is a highly non-local description of the fermions, although both completely eliminate the doubling. Susskinds method partially reduces the degeneracy and has the additional feature that the Euclidean formulation possesses a continuous axial symmetry which protects the theory from generating a fermion mass and which is known to be spontaneously broken in strong coupling with an accompanying Goldstone pion (Kluberg-Stern et al. 1983). The connection between doubling, the topology of the lattice and the Adler-Bell-Jackiw anomaly is expressed in the no-go theorem of Nielsen and Ninomiya (1981). The deep geometrical connection between Susskind fermions and Dirac-Kahler fermions is examined in some detail. The lattice and continuum versions of the Dirac-Kahler theory have the same fermion degeneracy and the continuum Dirac-Kahler equation may be diagonalized into four independent Dirac equations. The same diagonalization of the lattice Dirac-Kahler equation can only be done in momentum space, but not in coordinate

space where the flavours remain intertwined. Nevertheless this formulation enables us to explicitly identify the Susskind flavours in the continuum limit of the lattice theory in a meaningful way. We show how it is possible to give the flavours different masses and how these correspond to non-local mass terms (one-, two-, or three-link operators) for the lattice Susskind fermions. We then find the mass term that is most local on the lattice, since this will be the most practical to use in any simulation. We show how this mass term could be used in a simulation of QCD by an explicit identification of the lattice flavours with those of the real world. Alternatively, if we are only interested in light quarks it is possible to completely decouple the unwanted flavours by giving them masses of the order of the lattice cutoff.

The question of incorporating dynamical fermions into lattice gauge theories is then examined in chapter 3. A number of the proposals that have been put forward are discussed and their applicability to four dimensional simulations is examined. The anticommuting fermion degrees of freedom may be integrated out giving an effective action for the gauge field that can, at least in principle, be simulated by Monte Carlo techniques. However some approximation is necessary to make such simulations feasible, since the effective action couples all the gauge variables of the lattice. The pseudo-fermion method is introduced, in which small changes in the gauge field between successive configurations enables the change in the effective action between updates to be linearized. In this way the problem is reduced to one of evaluating the Green functions of the fermionic operator $(\not{\partial}+m)$ for neighbouring sites. The Metropolis pseudo-fermion method does this by a Monte Carlo over a

set of bosonic variables while the Langevin method evaluates the propagators by introducing a spurious "time" dependence and letting the pseudo-fermions evolve in the background gauge field according to the Langevin equation. The Langevin method is examined in both a first and second order formalism.

These techniques are tested in chapter 4 using the Schwinger model. We firstly review the essential features of the Schwinger model, and particularly those which are believed to be important in QCD. The Schwinger model was chosen because it both exhibits the property of confinement and because there are exact results for the massless model which serve as a check on the reliability of the techniques we wish to test. Various details of how the pseudo-fermion methods may be implemented and optimized are discussed and the results of the simulations using the Schwinger model are presented. It is found that the Langevin method is the faster of the two, although this is mainly as a result of the simplicity of the U(1) gauge group of the theory and would not be the case for theories like QCD where the link variables have many more parameters. Finally, we test the proposal of chapter 2 that unwanted flavours may be decoupled by giving them a mass of the order of the cutoff. We find that the measurements are in agreement with the one-species Schwinger model, whereas two degenerate flavours give results in agreement with the two-species model. The proposal that the unwanted flavours may be eliminated by only including half the fermionic contribution to the effective action is shown to fail in this instance. We also address the prediction of Coleman that there is an isospin symmetry in the SU(2) Schwinger model when both quarks are light and our results support this conclusion.

# CHAPTER 2

## FREE LATTICE FERMIONS

One of the major difficulties encountered in the description of fermions in lattice gauge theory is the proliferation of fermionic degrees of freedom in the continuum limit. Since we require the lattice theory to reproduce continuum physics in the limit that the lattice spacing tends to zero this doubling is rather problematic. A number of proposals (Wilson 1974; Drell et al. 1976; Susskind 1977) for overcoming this difficulty are examined and their various merits are discussed. The relationship between species doubling and chiral symmetry (Karsten and Smit 1981) is discussed, as is the no-go theorem of Neilsen and Ninomiya (1981). The intimate relation between species doubling and the geometric structure of the lattice, which is is elegantly displayed in the Kahler-Dirac formulation (Kahler 1962; Becher 1981), is reviewed in section 2. In particular, the equivalence between the Kahler-Dirac and Susskind formulations is discussed. These insights enable us, in section 3, to carry to fruition the idea (Susskind 1977; Banks et al. 1977) that the remaining degeneracy in the Kahler-Dirac-Susskind formulation may be interpreted as a flavour degeneracy (Burkitt, Kenway and Kenway 1983; Mitra 1983; Becher and Joos 1983; Kluberg-Stern et al. 1983). Indeed we show the identification explicitly and also how the different flavours may be given different masses. This idea will be pursued further (in chapter 4) as a means of removing unwanted fermions.

## 2.1 The Lattice Fermion Doubling Problem

The "naive" fermion action is obtained by a simple discretization of the usual Dirac action;

$$S_F = \frac{1}{2} \sum_{n,\mu} \bar{\psi}(n) \gamma_\mu \left[ \psi(n+\hat{\mu}) - \psi(n-\hat{\mu}) \right] + m \sum_n \bar{\psi}(n) \psi(n) \qquad (2.1)$$

where we neglect gauge fields for the moment (as we do throughout this chapter) and put the lattice spacing to unity. The $\bar{\psi}(n)$ and $\psi(n)$ are the usual Dirac spinors at every site of the lattice and the symmetric form of the difference operator is necessary in order to ensure its antihermiticity properties.

The momentum space propagator is found in the usual way by doing a (discrete) Fourier transformation and solving the Green function equation. The allowed momenta (now also discrete) lie in the Brillouin zone $-\frac{\pi}{a} < p < \frac{\pi}{a}$. The lattice propagator is then

$$\left[ m + \frac{1}{a} \sum_\mu i \gamma_\mu \sin p_\mu a \right]^{-1} \qquad (2.2)$$

This fermion propagator does not vanish in the limit $a \to 0$ in $2^d$ ($d$ being the dimensionality) regions of the Brillouin zone corresponding to the points $p_\mu = 0$ or $\frac{\pi}{a}$. Thus, even in a system which initially contains only particles corresponding to one pole, as soon as a gauge field is introduced the other allowed particles will be pair produced and consequently contribute to intermediate processes. For example, in a perturbation expansion all internal fermionic loops will contribute with a factor of $2^d$ times their counterparts in the continuum theory (Guerin and Kenway 1980; Sharatchandra, Thun and Weisz 1981). This is clearly unsatisfactory for Monte-Carlo

simulations since asymptotic freedom is lost for the SU(2) colour group and almost lost for SU(3).

A number of methods for avoiding this multiplicity of fermions have been proposed. One of these methods (SLAC fermions) (Drell, Weinstein and Yankielowicz 1976) entirely eliminates the doubling and maintains chiral invariance, but at the cost of locality. Since the doubling is intimately connected with the particular form of the lattice derivative, the method involves introducing a different gradient operator on the lattice from that used in eq.(2.1). Explicitly;

$$\begin{aligned} \partial_\mu \psi(n) &\equiv \sum_p i p_\mu e^{ip\cdot n} \psi(p) \\ &= \frac{1}{V} \sum_p i p_\mu e^{ip\cdot n} \sum_{n'} e^{-ip\cdot n'} \psi(n') \end{aligned} \tag{2.3}$$

where the sums on p and n are over the allowed momenta and sites respectively, V is the volume and we have set a=1, as we will do throughout. This expression shows clearly that the definition is non-local on the lattice, and moreover Lorentz invariance and locality are not restored in the continuum limit. Indeed, the one loop vacuum polarization diagram has been evaluated in perturbation theory and gives manifestly non-covariant results even in the continuum limit (Karsten and Smit 1979).

A method due to Wilson (1974) eliminates the doubling entirely by projecting away the unwanted fermions. Since it is only the continuum limit of the lattice theory that is physically interesting, we are free to add to the Lagrangian any terms which are of order the cutoff, since such terms will vanish in the continuum limit. In particular it is possible to add to the Lagrangian a term that is the

lattice version of the second derivative of the fermion field. The action then takes the form

$$S = \frac{1}{2}\sum_{n,\mu} \bar{\psi}(n)\left[(\gamma_\mu - r\mathbb{1})\psi(n+\hat{\mu}) - (\gamma_\mu + r\mathbb{1})\psi(n-\hat{\mu})\right] + m\sum_{n} \bar{\psi}(n)\psi(n) \tag{2.4}$$

where $\mathbb{1}$ is the unit matrix in spinor space. The Wilson parameter r gives the 15 unwanted fermions a mass m+2kr/a (k=1,2,3,4) and only one fermion remains in the continuum limit (corresponding to the point $p_\mu$=0 in the Brillouin zone). An alternative intuitive explanation of the effect of the Wilson parameter involves the projecting-out of components. Consider the case r=1 in which, choosing $\gamma_0$ to be diagonal,

$$\begin{aligned} \gamma_0 - \mathbb{1} &= \text{diag}(0,0,-2,-2) \\ \gamma_0 + \mathbb{1} &= \text{diag}(2,2,0,0) \end{aligned} \tag{2.5}$$

Thus two components in both the forward and the backward directions have been projected out. The Lagrangian (2.4) simply incorporates this feature in a way that maintains the Euclidean invariance. The resulting propagator is

$$\left[m + \sum_\mu i\gamma_\mu \sin p_\mu + r\sum_\mu (1-\cos p_\mu)\right]^{-1} \tag{2.6}$$

One disadvantage of Wilson fermions is that, unlike SLAC fermions, chiral ($\gamma_5$) symmetry is broken explicitly even for m=0. This represents a problem because chiral invariance is supposed to be an important approximate symmetry of QCD; one of the consequences of

which is the smallness of the pion mass. As a result the lack of chiral invariance in the continuum limit of lattice QCD will reflect directly on the value of the pion mass. In practice, what is done in a QCD lattice simulation is that the bare mass in the Wilson action is 'tuned' to give the correct pion mass in the continuum.

In the formulation of Susskind (1977) there is a hidden cubic symmetry which ensures that no such tuning of a quark mass parameter is necessary (Sharatchandra et al. 1981). Moreover the fermion degeneracy is reduced from $2^d$ to $2^{d/2}$ in d dimensions. In this method the fermion degrees of freedom are distributed around a unit cell. Indeed the original prescription consists of placing the different spinor components at different sites of the lattice. In two dimensions we can vizualise a 'staggered' lattice in which the upper spinor components sit on even sites, lower components on the odd sites of the lattice and the natural size of the unit cell is 2x2. The chiral symmetry now manifests itself as a discrete translational symmetry, which in this (two-dimensional) picture clearly interchanges the spinor components. The rationale behind this proposal comes from the observation that the original action can be rewritten as the sum of two identical terms on non-interacting sub-lattices. Susskinds prescription then tells us to simply throw away one of the redundant copies of the fermionic action. This decoupling of the action into identical copies can be carried out explicitly by the unitary transformation (Kawamoto and Smit 1981)

$$\psi(n) = (\gamma_1)^{n_1}(\gamma_2)^{n_2}(\gamma_3)^{n_3}(\gamma_4)^{n_4}\chi(n) \qquad (2.7)$$

where $n_i$ (i=1,2,3,4) are the components of the lattice site. (Note

that since this transformation is site dependent it has no continuum analogue and thus there is, of course, no such decoupling in the continuum). The Lagrangian, when rewritten in terms of the new fields $\chi(n)$, completely decouples into four identical spinor copies. By discarding three of the copies the degeneracy is reduced from sixteen to four in four-dimensions (and from four to two in two-dimensions). Using the expression (2.7) the action becomes

$$S = \frac{1}{2}\sum_{n,\mu} \bar{\chi}(n)\eta_\mu(n)\left[\chi(n+\hat{\mu}) - \chi(n-\hat{\mu})\right] + m\sum_n \bar{\chi}(n)\chi(n) \quad (2.8)$$

where $\eta_1(n)=1$, $\eta_2(n)=(-1)^{n_1}$, $\eta_3(n)=(-1)^{n_1+n_2}$, and $\eta_4(n)=(-1)^{n_1+n_2+n_3}$. This decoupling can, equivalently, be carried out in momentum space (Sharatchandra, Thun and Weisz 1981).

The propagator for Susskind fermions on an $N^4$ periodic lattice is given by

$$G(n,n') \equiv \langle \bar{\chi}(n)\chi(n')\rangle = \sum_{q_\mu=1}^{N} \exp\left(iq.(n'-n)\frac{\pi}{N}\right) \frac{\left\{m - i\sum_{\mu=1}^{4}\eta_\mu(n')\sin\left(q_\mu\frac{\pi}{N}\right)\right\}}{m^2 + \sum_{\mu=1}^{4}\sin^2\left(q_\mu\frac{\pi}{N}\right)} \quad (2.9)$$

where the $\eta_\mu(n)$ are as above. It is clear from this expression that translational invariance by one lattice unit is lost (as we would expect) but that the translational invariance of the unit cells $(2)^d$ is retained. Moreover, the poles in momentum space occur at exactly the same places ($q_\mu=0$ or $N$) as for the naive propagator, the difference being that the fermionic degrees of freedom have been thinned and a fermion is now spread over a number of neighbouring sites.

That none of the above methods fulfills our hopes of obtaining a lattice gauge theory with just one fermion and with continuous chiral invariance and a covariant continuum limit may appear rather unfortunate. However, the reason (Karsten and Smit 1981) is intimately connected with the Adler-Bell-Jackiw anomaly (Adler 1969; Bell and Jackiw 1969). The doubling occurs in such a way that even if we put a single left handed spinor on the lattice it would reappear doubled with a right handed counterpart in the continuum limit i.e. by regularizing a chiral lattice theory with a lattice cutoff and then removing the cutoff by taking the continuum limit $a \to 0$ we find that the theory contains an equal number of right and left handed fields and it is thus no longer chiral. This is perhaps not too surprising since it is well known in perturbation theory in the continuum that it is not possible to regularize a chiral theory in a chirally invariant manner. This connection between doubling and chirality is formalized in the Nielsen-Ninomiya theorem (1981), which is a no-go theorem for putting theories of the weak interaction on the lattice.

## 2.2 Dirac-Kahler Fermions

The geometric interpretation of the gluon field, describing infinitesimal parallel transports of the local colour coordinates, plays an important part in the formulation of the Wilson action for pure lattice gauge theories (Wilson 1974). However, in the formulations of the Dirac field on the lattice discussed in the previous section the geometric properties of spinors were completely disregarded. Indeed, the spinors were rather arbitrarily associated

with quantities defined on lattice points. In order to find a more consistent procedure, one should start with a geometric formulation of the Dirac equation. Such a geometric description of Dirac particles in the language of differential forms has been carried out by Kahler (1962) and recently rediscovered by a number of authors (Becher 1982; Rabin 1982; Banks et al. 1982) and applied to QCD by Becher and Joos (1982a,b). Both the continuum Dirac-Kahler equation and its lattice approximation exhibit the same flavour degeneracy. The multiplicity of states of given momentum of the Dirac-Kahler equation in D dimensions is, like the Susskind formulation, $2^{D/2}$ times that of the free Dirac equation. This similarity with Susskind fermions is more than accidental: the Susskind description of Dirac fields is equivalent to the lattice approximation of the Dirac-Kahler equation, as we will show shortly. In the continuum the reduction of the Dirac-Kahler equation into $2^{D/2}$ uncoupled Dirac equations occurs as a result of a decomposition of the underlying Clifford algebra. This decomposition can, equivalently, be expressed in terms of symmetry properties. However, on the lattice the decomposition is only possible in momentum space.

Our purpose here is to review the features of the Dirac-Kahler formulation that are important to our understanding of lattice fermions. The natural language of Dirac-Kahler fermions is that of differential forms and, although it is not our intention to provide a comprehensive guide to this formalism, a certain minimum will be useful for our purposes. First, we examine the continuum Dirac-Kahler equation, followed by its lattice version. The equivalence with Susskind fermions and the relationship to other lattice actions is described. Mention is also made of an equivalent

formulation due to Gliozzi (1982).

Differential forms provide a convenient notation for the differential calculus of antisymmetric tensor fields $A_{\mu_1 \ldots \mu_p}(x)$. Tensors of rank p are associated with p-forms $A_{|\mu_1 \ldots \mu_p|} dx^{\mu_1} \wedge \ldots \wedge dx^{\mu_p}$, where the $dx^\mu$ anticommute $dx^\mu \wedge dx^\nu = -dx^\nu \wedge dx^\mu$ and the notation $|\mu_1 \ldots \mu_p|$ means that only the terms with $\mu_1 < \mu_2 < \ldots < \mu_p$ are included in the sum ($\mu = 1, \ldots, D$). The first step is to translate the Euclidean Dirac equation

$$\left( \gamma^\mu \partial_\mu + m \right) \Psi = 0 \tag{2.10}$$

into the language of differential forms. At first sight this appears impossible because differential forms describe tensors, not spinors. However, it is possible to rewrite the above equation equivalently with $\Psi$ as a 4x4 matrix whose first column is $\Psi$ and whose other entries are zero. The equation then makes sense for any 4x4 matrix $\Psi$, and reduces to four independent Dirac equations, one for each column of $\Psi$, describing four uncoupled degenerate flavours. Since the $\gamma$ matrices and their products form a basis for 4x4 matrices, $\Psi$ can always be written uniquely as

$$\begin{aligned} \Psi(x) = {} & \chi_\phi(x) + \chi_\mu(x) \gamma^\mu + \frac{1}{2!} \chi_{\mu\nu}(x) \gamma^\mu \gamma^\nu \\ & + \frac{1}{3!} \chi_{\mu\nu\rho}(x) \gamma^\mu \gamma^\nu \gamma^\rho + \chi_{1234}(x) \gamma^1 \gamma^2 \gamma^3 \gamma^4 \end{aligned} \tag{2.11}$$

The Clifford algebra has a representation by differential forms, so $\Psi$ may be associated with

$$\Phi(x) = \chi_\emptyset(x) + \chi_\mu(x)dx^\mu + \frac{1}{2!}\chi_{\mu\nu}(x)dx^\mu \wedge dx^\nu + \frac{1}{3!}\chi_{\mu\nu\rho}dx^\mu \wedge dx^\nu \wedge dx^\rho + \chi_{1234}(x)dx^1 \wedge dx^2 \wedge dx^3 \wedge dx^4 \equiv \sum_H \chi_H(x)dx^H \tag{2.12}$$

The $2^d$=16 independent coefficients $\chi_H(x)$ are labelled by the ordered set of indices $H=(\mu_1,\ldots,\mu_k)$, $\mu_1<\mu_2<\ldots<\mu_k$ (including the empty set $\emptyset$), and $dx^H=dx^{\mu_1}\ldots dx^{\mu_k}$. In order to rewrite the Dirac equation we need the fundamental differential operator on forms. This generalized curl operator, denoted by d, converts p-forms to (p+1)-forms. In our notation

$$d\Phi = dx^\mu \wedge \partial_\mu \Phi = \sum_H \sum_\mu \rho_{\mu,H}\partial_\mu \chi_{H-\mu}(x)dx^H \tag{2.13}$$

where $\partial_\mu \Phi$ is the partial derivative of the coefficients $\chi_H(x)$ of $\Phi$. The sign factor $\rho_{\mu,H}$ is zero if $\mu$ does not belong to H, and is $(-1)^p$ if p is the number of transpositions required to commute $\mu$ in $H=(\mu_1,\ldots,\mu,\ldots,\mu_k)$ to the left. $H-\mu$ is the ordered set H without $\mu$. d has an adjoint operator $\delta$ which is the generalized divergence and which converts p-forms to (p-1)-forms. It is defined by a similar expression

$$\delta\Phi = -\sum_H \sum_\mu \rho'_{\mu,H}\partial_\mu \chi_{H\cup\mu}(x)dx^H \tag{2.14}$$

where the sign factor $\rho'_{\mu,H}$ is zero if $\mu$ belongs to H and is equal to $\rho_{\mu,H\cup\mu}$ otherwise. $H\cup\mu$ is the union of H with $\{\mu\}$ in natural order. The product of forms $\omega_1$ and $\omega_2$ is denoted by $\omega_1 \wedge \omega_2$ where the wedge product $\wedge$ is such that $dx^H \wedge dx^K = \rho_{H,K}dx^{H\cup K}$ if $H\cap K=\emptyset$ and

is zero otherwise.

The operators d and $\delta$ have the properties $d^2=0$, $\delta^2=0$, from which it follows that the Laplacian $\Box$ may be written as

$$\Box = (d-\delta)^2 = -(d\delta + \delta d) \tag{2.15}$$

$D=d-\delta$ is thus a natural square root of the Laplacian, a property which it shares with the Dirac operator $\gamma^\mu \partial_\mu$. The differential form $\Phi$ then satisfies the Dirac-Kahler equation:

$$(d-\delta+m)\,\Phi = 0 \tag{2.16}$$

which may be derived from the action

$$S = \frac{1}{4}\int \bar{\Phi}(d-\delta+m)\,\Phi \tag{2.17}$$

This action can be rewritten, using eq.(2.13) and eq.(2.14), as a sum of the Dirac actions of four independent flavours. The components in each of the columns of $\Phi$ are completely decoupled and remain decoupled when the minimal gauge field interaction is included in eq.(2.10). In order to establish the usual Dirac equation it is necessary to find an appropriate representation of the Clifford algebra. The existence of an associative Clifford product for differential forms (denoted by $\vee$ ) enables us to find such a representation. The Clifford product $\vee$ is defined for the basic elements $dx^\mu$ by

$$dx^\mu \vee dx^\nu = dx^\mu \wedge dx^\nu + g^{\mu\nu} \tag{2.18}$$

which clearly satisfies the defining relation of the $\gamma$ matrices:

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2 g^{\mu\nu} \tag{2.19}$$

However, the $\gamma$-matrix representation of the Clifford algebra in the 16 dimensional space of differential forms is reducible. As a result, the Dirac-Kahler equation decomposes into four identical copies of the usual Dirac equation. The linear transformation which accomplishes this decomposition is (Kahler 1962; Becher and Joos 1982a)

$$\begin{aligned} \psi_a^{(b)}(x) &= \frac{1}{2} \sum_H \Gamma_{ab}^H \chi_H(x) \\ \bar{\psi}_a^{(b)}(x) &= \frac{1}{2} \sum_H \Gamma_{ab}^{H^*} \bar{\chi}_H(x) \end{aligned} \tag{2.20}$$

where $\Gamma^H = \gamma_{\mu_1} \cdots \gamma_{\mu_k}$ (H as previously), $\Gamma^\emptyset = \mathbb{1}$ and $\psi^{(b)}$ ($b$=1,2,3,4) are the four uncoupled 'flavours' each obeying the Dirac equation (2.10). These four Dirac fields respect an SU(4) flavour symmetry, in analogy with the lattice case, and about which we will have more to say in the next section.

A notation for manipulating functions on a lattice can be set up in complete analogy to the notation of differential forms. The lattice analogue of p-forms are functions (called p-cochains) defined on p-dimensional hypercubes (called p-cells) in which vectors correspond to link variables, second rank tensors correspond to plaquette variables, etc.. This notation allows a straightforward

transcription of the Dirac-Kahler equation to the lattice:

$$\left(d\bar{} - \bar{\delta} + m\right) \overset{I}{\Phi} = 0 \qquad (2.21)$$

where, in this equation, $\overset{I}{\Phi}$ denotes a linear functional (p-cochain) defined on the elements (p-cells) of a (cubic) lattice: points (x), links $(x,\mu)$, plaquettes $(x,\mu,\nu)$, cubes $(x,\mu,\nu,\rho)$, etc.. One is free, of course, to reinterpret a p-cochain $A(x;\mu_1,\ldots,\mu_p)$ as a tensor-valued 0-cochain $A_{\mu_1\ldots\mu_p}(x)$. The 16 components of $\overset{I}{\Phi}$ may then be viewed as a 16 component fermion field defined on sites, although such a reinterpretation would obscure the geometrical information contained in $\overset{I}{\Phi}$. An analogy would be a gauge field $A_\mu(x)$ which can be regarded geometrically as a function on links or non-geometrically as four independent functions on sites. However, this analogy should not be pushed too far - particularly when we consider gauge transformations. The fact that some of the components of $\overset{I}{\Phi}$ are defined on links (for example) does not mean that they must be given the gauge transformation properties of a gauge field, because the geometry being discussed here is not related to the geometry one would introduce in adding gauge fields. Indeed, in gauging eq.(2.21) all the cochains $\chi_H(x)$ would be assigned the same transformation property under the local gauge transformation at x.

The differential operators $\bar{d}$ (dual boundary operator) and $\bar{\delta}$ (dual co-boundary operator) convert p-cochains to (p+1)- and (p-1)-cochains respectively:

$$\bar{d}\,\bar{\Phi} = \sum_{n,H}\sum_{\mu} \rho_{\mu,H}\,\Delta^{+}_{\mu}\,\chi_{H-\mu}(n)\,dx^{n,H}$$
$$\bar{\delta}\,\bar{\Phi} = -\sum_{n,H}\sum_{\mu} \rho'_{\mu,H}\,\Delta^{-}_{\mu}\,\chi_{H+\mu}(n)\,dx^{n,H} \qquad (2.22)$$

where $\Delta^{+}_{\mu}(\Delta^{-}_{\mu})$ is the forward (backward) derivative of the coefficients:

$$\Delta^{+}_{\mu}\chi_{H}(n) = \chi_{H}(n+\hat{\mu}) - \chi_{H}(n)$$
$$\Delta^{-}_{\mu}\chi_{H}(n) = \chi_{H}(n) - \chi_{H}(n-\hat{\mu}) \qquad (2.23)$$

As in the continuum the relations $\bar{d}^2=0$ and $\bar{\delta}^2=0$ ensure that

$$\Box = (\bar{d}-\bar{\delta})^2 = -(\bar{d}\bar{\delta} + \bar{\delta}\bar{d}) \qquad (2.24)$$

represents the correct lattice approximation to the Laplacian. The action for the lattice Dirac-Kahler fields is

$$S = \frac{1}{2}\sum_{n,H}\sum_{\mu} \bar{\chi}_{H}(n)\left\{\rho_{\mu,H}\left[\chi_{H-\mu}(n+\hat{\mu}) - \chi_{H-\mu}(n)\right]\right.$$
$$\left. - \rho'_{\mu,H}\left[\chi_{H+\mu}(n) - \chi_{H+\mu}(n-\hat{\mu})\right]\right\} \qquad (2.25)$$

It is straightforward to check that the energy-momentum spectrum of the Dirac-Kahler equation is qualitatively the same on the lattice as it is in the continuum and both versions have an overall four-fold degeneracy. However, when we try to carry out the reduction to the usual Dirac equation, in analogy with the continuum reduction, the relations cannot be expressed locally on the lattice. Indeed the flavour transformations have become intertwined with the translations and the lattice reduction in coordinate space is not possible. By

transforming to momentum space it is possible to carry out the diagonalization into four equivalent Dirac flavours, but the transformation back to coordinate space is non-local. How the flavours may be meaningfully identified in the lattice model (Burkitt, Kenway and Kenway 1983; Mitra 1983; Kluberg-Stern et al. 1983) is explained in the next section.

The equivalence between Dirac-Kahler and Susskind fermions (Dhar and Shanker 1982; Becher and Joos 1982) can be established straightforwardly by a simple relabelling of the fields. We define a new sublattice with a lattice spacing of half the original lattice and a new field $\chi(n)$ on this lattice. Then, in the notation used above,

$$\chi_H(n) \equiv \chi(2n + \hat{\mu}_1 + \ldots + \hat{\mu}_4) \qquad (2.26)$$

Thus the new $\chi$ field is simply the field $\chi_H(n)$ distributed over the corners of the unit cell on the new sublattice. This sublattice may be thought of as the lattice on which the p-cochains live since the above identification associates each p-cochain on the original lattice with its geometric centre, which is a site of the sublattice. The action (2.25), when re-expressed in terms of the $\chi$ fields, becomes exactly the Susskind action (2.8) on the sublattice.

Although the free-fermion Susskind and Dirac-Kahler theories are equivalent, the same is not true when gauge fields are introduced. The Susskind field is defined on a lattice with half the lattice spacing and 16 times the number of links, meaning that the density of gauge field degrees of freedom is 16 times greater than for the Dirac-Kahler formulation. In the Susskind formulation the different

spinor components of a fermion will transform differently under gauge transformations. The symmetries that result from such allowed transformations have important consequences when we consider mass counterterms.

An equivalent formalism for transforming the one-component Susskind theory into a version with four conventional Dirac spinors (Gliozzi 1982) is illuminating. In this version matrices, rather than cochains, are associated with the new blocked lattice sites (i.e. unit cells on the original lattice) and the action has a term which partially lifts the 16-fold naive fermion degeneracy in a way not unlike that of Wilson. It was observed that the action (2.1) is invariant under a discrete group of transformations generated by

$$\psi(n) \longrightarrow i(-1)^{n_\mu} \gamma_5 \gamma_\mu \psi(n)$$
$$\bar{\psi}(n) \longrightarrow -i(-1)^{n_\mu} \bar{\psi}(n) \gamma_\mu \gamma_5 \qquad (2.27)$$

Susskinds method is equivalent to a maximal diagonalization of this symmetry, of which the transformation (2.7) is one possible choice. A representation of $\gamma$ matrices is then built up in the space of one component spinors. The matrix notation is essentially that which emerges naturally in the next section.

## 2.3 Identification of Flavours

In order to examine the low energy behaviour of QCD it is necessary to have, in any lattice theory, at least the two light quarks (u and d) and perhaps also, with substantially heavier masses, the quarks s,c,... Since the Susskind-Dirac-Kahler fermion

formulation automatically gives a fourfold degeneracy it is natural in the context of realistic lattice calculations to regard these four species as the four fermion flavours u,d,c,s in the real world. Such a scheme would not contain any unphysical quark degrees of freedom (in contrast to the Wilson formulation where the unphysical fermion degrees of freedom only disappear in the continuum). However, this identification can only be realistic if we modify the lattice action by including a fermion mass term which will break their degeneracy. In the previous section it was pointed out that the lattice Susskind-Dirac-Kahler action for free fermions cannot be decomposed into a sum of lattice Dirac actions for four uncoupled flavours. However it is possible, as we shall show, to make the identification in the continuum limit of the lattice theory, and mass terms for the different flavours can then be constructed (Burkitt, Kenway and Kenway 1983; Mitra 1983; Kluberg-Stern et al. 1983; Becher and Joos 1982b). This lattice identification is ambiguous up to terms which are irrelevant in the continuum limit i.e. there are different lattice mass terms with the same continuum limit (Burkitt, Kenway and Kenway 1983).

This ambiguity only becomes important when we impose local gauge invariance. Then the Dirac-Kahler and Susskind lattice actions differ (in the ratio of the densities of the gauge to fermion degrees of freedom). In the former the continuum mass term translates into an effectively local lattice operator and so all lattice mass terms are equally good for doing calculations (from both speed and accuracy considerations). The Susskind formulation maintains the spatial distribution of Dirac-Kahler fields so the continuum mass term translates into a non-local lattice fermion operator (unless all four

flavours are degenerate), which must be made gauge invariant by including the appropriate string of gauge fields on links. So, from amongst the different lattice mass terms, we may seek the most local one as the best for calculations. This means that there is an optimum identification between lattice and continuum fields within the Susskind formulation such that the lattice QCD action with four non-degenerate flavours is as local as possible. A scheme is presented here in which the SU(4) flavour symmetry is broken to SU(2) using only a one-link operator. The resulting lattice action is no more non-local than when all four flavours are degenerate and so is well within the capability of existing Monte-Carlo simulation schemes. Further flavour symmetry breaking, even within this optimum scheme requires two- and three-link lattice operators and so is much harder to implement in practice. The relationships between the various possible mass terms and masses induced by quantum corrections are also investigated. The two-dimensional case is investigated in some detail and the propagators for the Susskind field $\chi$ and the physical particles are given explicitly. The scheme presented here has been applied to the one- and two-species Schwinger models (Burkitt and Kenway 1983) and the results are presented in chapter 4.

In order to identify the flavours of the Susskind action eq.(2.8) we use the identification with Dirac-Kahler fermions of eq.(2.26) and the associated notation. In the continuum the transformation which accomplishes the decomposition of the Dirac-Kahler action into four uncoupled Dirac actions is given by eq.(2.20). It is important to notice that this transformation depends on the representation chosen for the $\gamma$-matrices. We extend this transformation to the lattice theory.

The continuum mass term, giving mass $m_b$ to flavour b, is, using eq.(2.20)

$$\int d^4x \sum_{b=1}^{4} m_b \psi^{(b)\dagger}(x) \psi^{(b)}(x) = \int d^4x \, \chi_H^\dagger(x) M_{HK} \chi_K(x) \qquad (2.28)$$

where the 16x16 matrix

$$M_{HK} = \frac{1}{4} Tr \left[ \Gamma^K M (\Gamma^H)^\dagger \right] \qquad (2.29)$$

and

$$M = \sum_{b=1}^{4} m_b \rho^{(b)} \quad , \quad \rho^{(b)}_{cd} = \delta_{cb} \delta_{db} \qquad (2.30)$$

depends on the representation of the $\gamma$-matrices. In the Weyl basis,

$$\gamma_j = i \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix} \quad , \quad \gamma_4 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \qquad (2.31)$$

where $\sigma_j$ , $j=1,2,3$ are the Pauli matrices.

$$M_{weyl} = \frac{1}{4} \Big\{ \mathbb{1} (m_1+m_2+m_3+m_4) - i\gamma_1\gamma_2 (m_1-m_2+m_3-m_4) \qquad (2.32)$$
$$- i\gamma_3\gamma_4 (m_1-m_2-m_3+m_4) - \gamma_1\gamma_2\gamma_3\gamma_4 (m_1+m_2-m_3-m_4) \Big\}$$

We propose to use expressions analogous to eq.(2.28)-(2.30) for the lattice theory. Then M's corresponding to different $\gamma$-matrix representations (equivalent in the continuum) give inequivalent lattice mass terms. The Dirac-Kahler lattice theory has all sixteen fields $\chi_H(n)$ transforming the same way under local gauge transformations. So the lattice mass term

$$\sum_n \bar{\chi}_H(n)\, M_{HK}\, \chi_K(n) \tag{2.33}$$

is automatically gauge invariant and, although different $\gamma$-matrix representations give different lattice actions, they are all equally good for doing calculations. In contrast, because of eq.(2.26), the corresponding Susskind lattice mass term behaves as a non-local operator under gauge transformations, and is made gauge invariant by introducing a string of gauge fields on the links joining $\bar{\chi}_H(n)$ and $\chi_K(n)$. For example, in the Weyl basis eq.(2.32) leads to two- and four-link lattice operators if all the flavours have different masses.

It follows that there may be an alternative representation for the $\gamma$-matrices which leads to a more local lattice mass term. This amounts to finding an alternative to the 'reduction' group of Becher and Joos (1982a,b): $\{1, i\gamma_1\gamma_2, i\gamma_3\gamma_4, \gamma_1\gamma_2\gamma_3\gamma_4\} = Z_2 \times Z_2$ employed in eq.(2.32). The best choice is $\{1, \gamma_2, i\gamma_3\gamma_4, i\gamma_2\gamma_3\gamma_4\}$ which corresponds to choosing $\gamma_2$ diagonal. The resulting mass term has

$$M = \tfrac{1}{4}\{\mathbb{1}(m_1+m_2+m_3+m_4) + \gamma_2(m_1+m_2-m_3-m_4) \tag{2.34}$$
$$+ i\gamma_3\gamma_4(m_1-m_2-m_3+m_4) + i\gamma_2\gamma_3\gamma_4(m_1-m_2+m_3-m_4)\}$$

and consequently leads to one-, two- and three-link lattice operators. That this is the best we can do follows from the fact that any reduction group, isomorphic to $Z_2 \times Z_2$, can contain at most one of $\gamma_\mu$, $\mu = 1,2,3,4$ and $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4$.

Thus this $\gamma$-matrix representation and the corresponding flavour identification (2.20) provides the optimum formulation of lattice QCD

using Susskind fermions, in the sense of being the most local if the flavours are given different masses. In particular, it follows from (2.33) and (2.34) that SU(4) flavour can be broken to SU(2) isospin by setting $m_1=m_2<<m_3=m_4$ and the resulting lattice gauge theory contains at most one-link fermion operators (these are the terms that are needed in the calculation of the lattice derivative in any case).

In chapter 4 we apply this proposal for giving different masses to the Susskind flavours to a simulation of the Schwinger model (two-dimensional QED). The possibility of decoupling unwanted flavours by giving them a mass of the order of the cutoff will also be investigated. It is thus useful to illustrate explicitly how the formalism discussed above may be used in a two-dimensional calculation. On a 2Nx2N Euclidean space-time lattice (the simulations were carried out on a 64x64 lattice, i.e. N=32) with periodic boundary conditions the Susskind action for free massless fermions is

$$S_F^{(0)} = \frac{1}{2}\sum_{\underline{n}=(1,1)}^{(2N,2N)} \bar{\chi}(\underline{n})\Big\{\chi(\underline{n}+\underline{e}_1) - \chi(\underline{n}-\underline{e}_1) + (-1)^{n_1}\left[\chi(\underline{n}+\underline{e}_2) - \chi(\underline{n}-\underline{e}_2)\right]\Big\} \tag{2.35}$$

where $\bar{\chi}(\underline{n})$ and $\chi(\underline{n})$ are one component fermion fields and $\underline{e}_\mu (\mu=1,2)$ are the lattice unit vectors. In the continuum limit $S_F^{(0)}$ describes two massless flavours u and d. Introducing masses for the two flavours by eq.(2.29) and (2.33) gives the action

$$S_F = S_F^{(0)} + \frac{1}{2}\sum_{\underline{n}=(1,1)}^{(N,N)} \bar{\chi}_H(\underline{n})\, Tr\left(\Gamma^K M \Gamma^{H\dagger}\right)\chi_K(\underline{n}) \tag{2.36}$$

where $\Gamma^\emptyset = 1$, $\Gamma^1=\gamma_1$, $\Gamma^2=\gamma_2$ and $\Gamma^{12}=\gamma_1\gamma_2$ with $\{\gamma_\mu,\gamma_\nu\}=2\delta_{\mu\nu}$,

$\gamma_\mu^\dagger = \gamma_\mu$, is a complete set of four Euclidean gamma matrices (note that the summation is now on the block lattice). M in eq.(2.36) depends on the representation of the gamma matrices and the most local mass term results from choosing $\gamma_2$ (equivalently $\gamma_1$) diagonal. Then

$$M = \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix} = \frac{1}{2}\left[\mathbb{1}(m_u + m_d) + \gamma_2 (m_u - m_d)\right] \tag{2.37}$$

where $m_u, m_d$ are the masses of flavours u, d in lattice units. On the original lattice (of spacing 1), eq.(2.36) is

$$\begin{aligned} S_F = S_F^{(0)} &+ \frac{m_u + m_d}{2} \sum_{\underline{n}=(1,1)}^{(2N,2N)} \bar{\chi}(\underline{n})\chi(\underline{n}) \\ &+ \frac{m_u - m_d}{4} \sum_{\underline{n}=(1,1)}^{(2N,2N)} \Big\{\left[1+(-1)^{n_2}\right]\bar{\chi}(\underline{n})\chi(\underline{n}+\underline{e}_2) \\ &\qquad + \left[1-(-1)^{n_2}\right]\bar{\chi}(\underline{n})\chi(\underline{n}-\underline{e}_2)\Big\} \end{aligned} \tag{2.38}$$

For the case $m=m_u=m_d\neq 0$ the propagator is given by eq.(2.9) (with the sum over $\mu=1,2$ only). Since we shall be measuring the expectation values $\langle\bar{u}u\rangle$ and $\langle\bar{d}d\rangle$ (in chapter 4), which are the diagonal elements of the propagators, we give their explicit form for $m=m_u=m_d\neq 0$

$$\begin{aligned} \frac{1}{2}\left(\langle\bar{u}u\rangle + \langle\bar{d}d\rangle\right) &= \frac{1}{2}\,\frac{1}{(2N)^2} \sum_{\underline{n}=(1,1)}^{(2N,2N)} \bar{\chi}(\underline{n})\chi(\underline{n}) \\ &= \frac{m}{2N^2} \sum_{\underline{q}=(1,1)}^{(N,N)} \frac{1}{m^2 + \sin^2\frac{q_1\pi}{N} + \sin^2\frac{q_2\pi}{N}} \end{aligned} \tag{2.39}$$

which is plotted as a function of the fermion mass in Figure 1 for $2N=64$. The divergence as $m\to 0$ is a finite size effect and indicates

that we can trust our calculations for m>0.03.

The analytic expression for the lattice propagator when $0<m_u<m_d$ is too complicated to present here and its explicit form is not very enlightening, but we have used it to calculate

$$\langle\bar{u}u\rangle = \frac{1}{2}\frac{1}{(2N)^2}\sum_{n=(1,1)}^{(2N,2N)}\Big\{\bar{\chi}(n)\chi(n) + \frac{1}{2}\left[1+(-1)^{n_2}\right]\bar{\chi}(n)\chi(n+e_2) + \frac{1}{2}\left[1-(-1)^{n_2}\right]\bar{\chi}(n)\chi(n-e_2) \qquad (2.40)$$

as a function of $m_u$ for $m_d=1$ and the result is shown graphically in Figure 1.

The relationship between the $\bar{\chi}(n)$ and $\chi(n)$ that sit on the sites of the lattice of spacing 1, and the physical u and d degrees of freedom which live on the blocked lattice (by which is meant the lattice of spacing 2) requires some elucidation. To go from the original lattice to the blocked lattice requires that we reformulate the theory in terms of variables that live on the sites of the block lattice, as has been done explicitly in eq.(2.39) where the final sum is over the allowed momenta of the blocked lattice. It is clear from eq.(2.20) and (2.26) that the spinor and flavour degrees of freedom of the physical fields have both become distributed over the unit cells of the small lattice. This has important consequences when gauge fields are introduced since we have the freedom to introduce the gauge field on either the original or the blocked lattice. With the one-component $\chi$ fields on the original lattice the action is

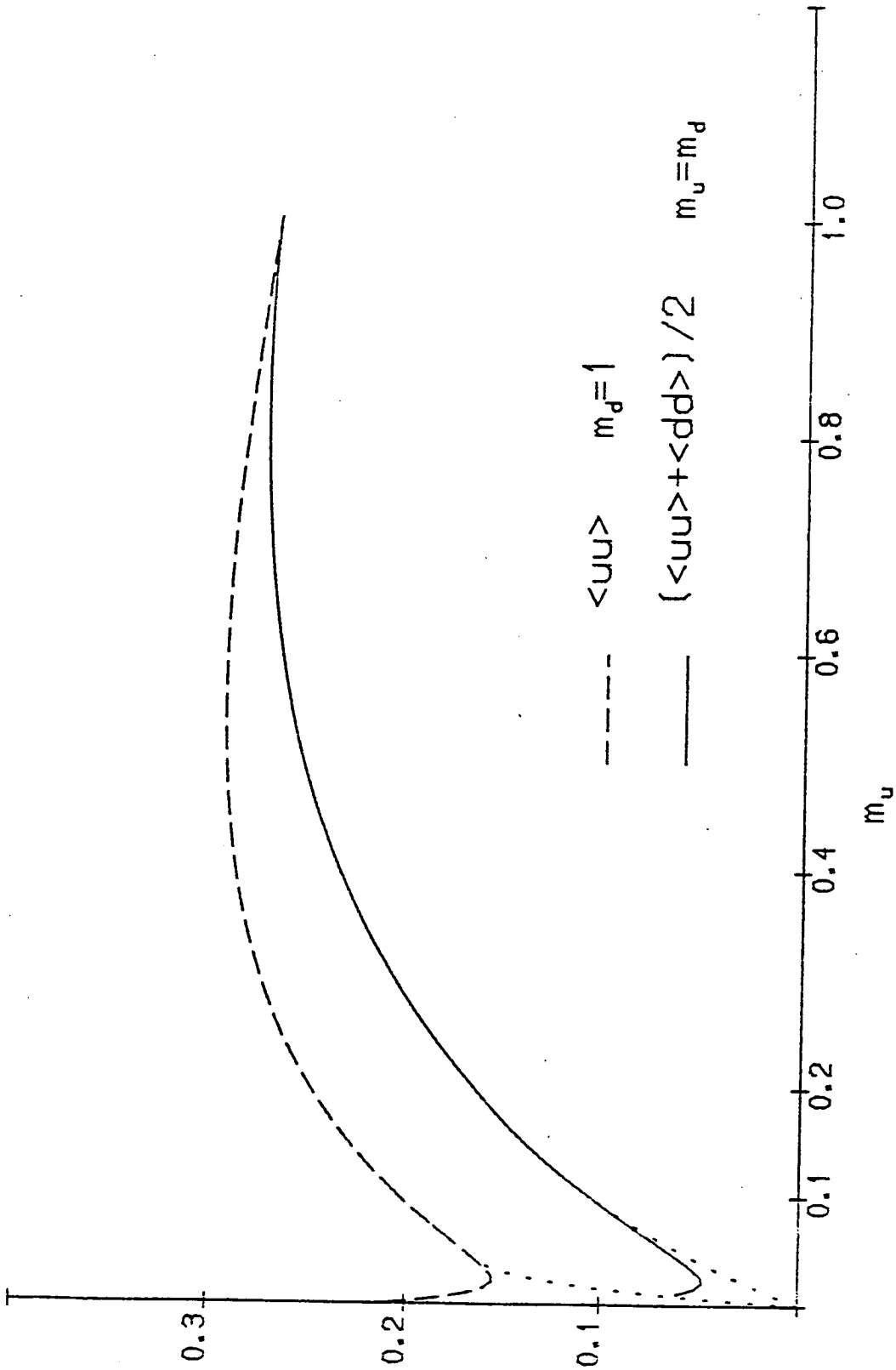



Figure 1 : Free Susskind fermions on 64x64 lattice. The dotted lines are the infinite lattice results.

$$S_F = \frac{1}{2}\sum_{n,\mu}\bar{\chi}(n)\eta_\mu(n)\left[U_\mu(n)\chi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\chi(n-\hat{\mu})\right] + m\sum_n \bar{\chi}(n)\chi(n) \tag{2.41}$$

and the associated free propagator is given by eq.(2.9). On the blocked lattice when we transform the $\chi_H$ fields to the $\psi$ fields through eq.(2.20) the action becomes

$$S_F = \frac{1}{2}\sum_{n,\mu}\bar{\psi}(n)\left[A_\mu \nabla_\mu \psi(n) + B_\mu \Delta_\mu \psi(n)\right] + \sum_n \bar{\psi}(n) M \psi(n) \tag{2.42}$$

where the mass term is given by eq.(2.34) and we define

$$\nabla_\mu \psi(n) = \left\{U_\mu(n)\psi(n+\hat{\mu}) - U_\mu^\dagger(n-\hat{\mu})\psi(n-\hat{\mu})\right\} \tag{2.43}$$

$$\Delta_\mu \psi(n) = \left\{U_\mu(n)\psi(n+\hat{\mu}) - 2\psi(n) + U_\mu^\dagger(n-\hat{\mu})\psi(n-\hat{\mu})\right\}$$

$A_\mu$ and $B_\mu$ are the following matrices:

$$A_\mu \equiv \gamma_\mu \otimes \mathbb{1}$$
$$B_\mu \equiv \gamma_5 \otimes \gamma_\mu\gamma_5 \tag{2.44}$$

where the first (resp. second) matrix in the tensorial products acts on spinor (resp. flavour) indices. The second term in eq.(2.42) distinguishes it from the naive action and couples the different flavours on the lattice, although it vanishes in the continuum limit. The (free) momentum space propagator of the action (2.42) with degenerate masses is (Kluberg-Stern et al. 1983)

$$\tilde{G}(p) = \frac{i\sum_\mu \sin(2p_\mu)(\gamma_\mu \otimes \mathbb{1}) + \sum_\mu (\cos 2p_\mu - 1)(\gamma_5 \otimes \gamma_\mu \gamma_5) - 2im\, \mathbb{1} \otimes \mathbb{1}}{2\left(m^2 + \sum_\mu \sin^2 p_\mu\right)} \quad (2.45)$$

The different symmetries possessed by the two actions are crucial when we consider mass counterterms in the interacting theory. The Susskind action (2.41) with degenerate masses has a continuous $\gamma_5 \otimes \gamma_5$ symmetry that is spontaneously broken at strong coupling, and there is a Goldstone pion (Kluberg-Stern et al. 1983). This appears to persist into the weak coupling regime where Sharatchandra et al. (1981) have shown that there is a cubic symmetry which prevents the generation of mass counterterms. However, the Dirac-Kahler action has a continuous $\gamma_5 \otimes \gamma_5$ symmetry that is not broken at strong coupling (Napoly 1983) and likewise at weak coupling it has been shown (Mitra and Weisz 1983) that there is no symmetry that prevents quark mass generation. Consequently to obtain zero quark masses in the Dirac-Kahler formalism it is necessary to tune the bare quark masses, in the same way as with Wilson fermions. Since the mass term we introduce breaks the symmetry of the Susskind action, quark masses will also be generated and a tuning of the bare quark masses is necessary.

# CHAPTER 3

# DYNAMICAL FERMIONS

## 3.1 Methods for Dynamical Fermions

Having discussed the problem of how to describe fermions on a lattice the question then becomes one of how to include them dynamically in lattice gauge theory calculations. The introduction of anticommuting variables is wellnigh impossible in a computer simulation since, on a lattice with N sites, the N anticommuting variables span an algebra with $2^N$ generators. For more than two dimensions it is thus entirely impracticable to introduce fermions directly and it is necessary to devise some appropriate approximation in order to be able to obtain useful results within acceptable computer time.

The standard Euclidean action bilinear in the fermionic variables is

$$S(\bar{\psi}, \psi, U) = S_G(U) + \sum_{I,J} \bar{\psi}_I M_{IJ}(U) \psi_J \qquad (3.1)$$

where $S_G(U)$ is the usual pure gauge action, subscripts I,J label sites of the lattice, and $M_{IJ}(U)$ is the lattice version of the Dirac operator $\not{\partial}+m$ (which will depend upon how we choose to describe the fermions on the lattice). Most calculations in lattice gauge theory to date have been done in the quenched approximation in which the fermionic contribution to the action (3.1) is neglected and the quarks treated as external sources. This approximation is equivalent to ignoring all internal quark loops in Feynman diagrams and gives an

exact Zweig rule. It is argued that internal quark loops should not be very important otherwise exotic components such as $qq\bar{q}\bar{q}$ would be important in meson spectroscopy.

In order to go beyond the quenched approximation and incorporate the fermionic degrees of freedom, which are believed to be important in the physical world, the first step is to eliminate the Grassmann variables. This may be done by analytically integrating out the fermionic variables using the standard Matthews-Salam formulae (Matthews and Salam 1954,1955)

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\{-S(\bar{\psi},\psi,U)\} = \det\{M(U)\}\exp\{-S_G(U)\}$$

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi\, \bar{\psi}_I \psi_J \exp\{-S(\bar{\psi},\psi,U)\} = M^{-1}_{JI}(U)\det\{M(U)\}\exp\{-S_G(U)\} \tag{3.2}$$

where the second expression describes the propagation of a quark in the background field U. These identities are clearly sufficient to enable us to eliminate the fermionic variables from any functional integral. Moreover the resulting bosonic gauge field integral is amenable, at least in principle, to standard Monte Carlo techniques. However, although the Matthews-Salam determinant is of the huge matrix M(U) and numerical calculation is still enormously difficult, the fact that the matrix has very few off diagonal elements is of crucial importance in any scheme. The gauge field in eq.(3.2) is thus generated with a probability distribution that is now governed not just by the pure gauge action $S_G(U)$ but by a new effective action to which the effect of fermionic loops contributes:

$$S_{eff}(U) = S_G(U) - Tr\,\ln M(U) \qquad (3.3)$$

$$= S_G(U) - \tfrac{1}{2} Tr\,\ln K(U)$$

where $K(U)=\overline{M}(U)M(U)$ is clearly hermitian and positive definite (it is the lattice version of the Klein-Gordon operator $-\not{\partial}^2+m^2$).

A variety of techniques based on the effective action have been discussed in the literature and applied to various models. In this chapter some of these techniques will be examined, particularly with a view towards their viability in an unquenched simulation of four dimensional QCD. Practical aspects concerning the implementation of the methods on a computer are also discussed, particularly with a view towards the possibility of some sort of vector or parallel processing since such considerations are becoming increasingly important in large scale simulations of the sort used in lattice gauge theory. In the next section the pseudo-fermion method of Fucito, Marinari, Parisi and Rebbi (1981) will be examined in detail. By considering small variations ($\delta U$) in the gauge field between successive Monte Carlo iterations the change in the effective action of the gauge field (3.3) may be linearized (with respect to $\delta U$). The resulting Green functions for the fermionic action may then be approximated by a further Monte Carlo integration over bosonic variables, which are called pseudo-fermions. Alternatively, the Green functions may be approximated by iterating a Langevin equation (Parisi 1981; Fucito and Marinari 1981) and the resulting estimates fed back into the effective action to generate the subsequent gauge field configuration. Two versions of the Langevin algorithm are

examined and in the next chapter these techniques are applied to the Schwinger model and their relative usefulness evaluated.

The hopping parameter expansion (Lang and Nicolai 1982; Hasenfratz and Hasenfratz 1981) is in many respects analogous to the high temperature series expansion used in critical phenomena. The method has already been used in combination with an ordinary Monte Carlo simulation of the gauge fields in calculations of the SU(3) hadron spectrum (Hasenfratz, Hasenfratz, Kunszt and Lang, 1982a,b) The hopping parameter K is proportional to the amplitude for moving a quark by one lattice unit, and the order of the expansion is the length of the quark paths in lattice units. In the hadron mass calculations the masses are extracted by finding poles in the hopping parameter, as identified by Padé approximants, and relating them to singularities in the momentum space particle propagators. So long as the order of the expansion is compatible with the size of the hadron the results will be reasonably reliable. A simple example illustrates the main features of the method: the case of a free scalar field. On a lattice of spacing a the action is

$$S = \frac{-a^2}{2} \sum_{n,\mu} \left(\varphi(n+\mu)-\varphi(n)\right)^2 - \frac{a^4}{2} \sum_{n} m^2 \varphi^2(n) \qquad (3.4)$$

After a finite renormalization of the field $\varphi$ by $\varphi \to \sqrt{(8a^2+m^2a^4)}\,\varphi$

$$\begin{aligned} S &= -\frac{1}{2} \sum_{n} \varphi^2(n) + K \sum_{n,\mu} \varphi(n)\varphi(n+\mu) \\ &\equiv \sum_{n,n'} \varphi(n) \Delta(n,n') \varphi(n') \end{aligned} \qquad (3.5)$$

where $K=a^2/(8a^2+m^2a^4)$ is the hopping parameter. The propagator is

simply the reciprocal of the operator $\Delta$ and can be found straightforwardly from the Green function equation

$$G(n,n') = \sum_{p_\mu} e^{-ip\cdot(n-n')}\,\tilde{G}(p)$$

$$\tilde{G}(p) = \left[1 - K\sum_{\mu}\left(e^{ip\cdot a} + e^{-ip\cdot a}\right)\right]^{-1} \qquad (3.6)$$

where the sum is over the allowed momenta. This propagator now has a simple diagrammatic expansion in K in which the elements are nearest-neighbour links. For each link there is a factor $Ke^{\pm p_\mu a}$ where $\mu$ is the direction of the axis of the link, and $\pm$ corresponds to the orientation of the link. The expansion of the propagator is the sum of all connected diagrams consisting of a single line of any length and any location starting from the origin. In the case where K is very small the expansion converges very quickly and only the lowest order diagrams are important. However it is easy to check that this does not give relativistic results. Indeed if we do the usual particle identification we find a particle of mass $a^{-1}\ell n(1/K)$, which is much larger than the cutoff $a^{-1}$. In the continuum limit $a\to 0$ (i.e. K near 1/8):

$$\tilde{G}(p) = \left[1 - 8K - KE^2a^2 + Kp^2a^2 + O(a^4)\right]^{-1}$$

$$\simeq \frac{Ka^2}{\frac{1-8K}{Ka^2} + p^2 - E^2} \qquad (3.7)$$

and we find that the pole in the propagator occurs for $E(p)=\sqrt{m^2+p^2}$ where the mass is given by $m^2=(1-8K)/Ka^2$, as we would expect. This simple example illustrates the principle features of the method

although in practice we will only know the expansion in K to some finite order, which will contain not only the pole term but also an approximation to the branch cuts by sequences of poles and zeros and very high orders are needed to separate the particle pole. In interacting theories the number of terms grows rapidly as the order of the expansion is increased and the method is not practical if the correlation length is large. In a gauge theory the situation is naturally more complicated since each link has associated with it a factor $K(1-\gamma_\mu)U_\mu(n)$ (or $K(1+\gamma_\mu)U_\mu(n)$ when traversing links in the opposite direction), and the trace is taken in Dirac, colour and flavour space with the usual factor of -1 associated with fermion loops. In the hadron mass calculations of Hasenfratz, Hasenfratz, Kunszt and Lang (1982a,b) the relevant propagators were expanded in powers of K, corresponding to Wilson loops of various lengths. The Wilson loop expectation values were determined by ordinary Monte Carlo on an $8^4$ lattice. The series obtained for mesons and baryons were of $10^{th}$ and $12^{th}$ order respectively, but were judged too short to make a reliable analysis.

Another related method has been proposed by Kuti (1982). Instead of systematically drawing all the paths order by order, they are generated stochastically. A local change in the gauge field $U \rightarrow U+\delta U$ implies (Scalapino and Sugar 1981)

$$\frac{\exp[-S_{\text{eff}}(U+\delta U)]}{\exp[-S_{\text{eff}}(U)]} = \det[1+M^{-1}(U)\delta M]\frac{\exp[-S_G(U+\delta U)]}{\exp[-S_G(U)]} \qquad (3.8)$$

where $\delta M$ is the resulting change in the matrix M. With local boson-fermion coupling the non-trivial change $\delta M$ in the fermion

matrix is restricted to the neighbourhood of the updated lattice site(s) and thus only a limited number of elements of $M^{-1}$ are required at each Monte-Carlo step. The method is essentially an efficient technique for the approximate summation of the von Neumann series defined by the inverse of the operator M and it involves considering a random walk in the domain of integers. The walk begins at some selected point i, proceeds from point to point with certain transition probabilities and terminates at some point j with a given stop probability. The inverse matrix elements $M_{ij}$ are then related to the transition and stop probabilities. The main problem in any serious application is to correctly choose the transition probabilities. If they are not correctly chosen then most of the time is spent generating irrelevant paths and the convergence will be slow. For a given statistical accuracy the number of walks required does not depend upon the size of the matrix and consequently the update time is not dependent on the lattice volume. The method has been shown to be effective on a simplified four dimensional model and work is underway to apply it to non-Abelian gauge theories.

A method due to Scalapino and Sugar (1981) involves an updating of both the gauge field configuration $\{U\}$ and all the inverse matrix elements $M^{-1}$. It uses the fact that a change in a gauge variable on some link k will induce a change in $M_{ij}$ only for values of i and j in the vicinity of k. As a result $\delta M_{ij}(U)$ is nonzero only for a small number (L) of values of i and j and in order to obtain the determinant factor of eq.(3.8) only the determinant of an LxL matrix need be calculated. The values for the entire matrix $M^{-1}(U)$ are stored between iterations and updated according to the scheme

$$(M+\delta M)^{-1}_{ij} = M^{-1}_{ij} - \frac{M^{-1}_{ik}\,\delta M_{kl}\,M^{-1}_{lj}}{1+\delta M_{kl}\,M^{-1}_{lk}} \qquad (3.9)$$

which is an exact identity and the indices k and l are summed over the L non-vanishing values of $\delta M_{kl}$. Rounding errors, which will cause $M^{-1}$ to stray from its true value after many iterations, may be eliminated by carrying out a correction procedure after so many iterations. This is typically done by replacing $M^{-1}$ by $2M^{-1}-M^{-1}MM^{-1}$, which essentially renormalizes the product $M^{-1}M$ to unity and in practice reduces the fluctuations to the order of the machine noise. This algorithm has been shown to work for a simple one dimensional model (Scalapino and Sugar 1981) and the Schwinger model (Duncan and Furman 1981), where the Wilson loop behaviour was calculated and shown to be consistent with the perimeter law, as we would expect when dynamical fermions are included, although the lattice was too small (12x12) to give definitive results. Chiral correlation functions were also measured, although primarily as a means of investigating the (large) edge effects. The method is limited by the huge times required to calculate the entire matrix $M^{-1}$ and the associated memory requirements, and consequently it does not appear to be viable for four dimensional lattices of reasonable size.

The calculation of the fermionic determinant can also be reduced to the problem of calculating $M^{-1}(U)$ in a different way. If we write $M(U)=1-KB(U)$, where K is the usual hopping parameter, and consider a system of two identical fermion flavours then the fermionic contribution to the effective action may be written as

$$[\det(1-KB)]^2 = \int \mathcal{D}Q \exp\{-\tfrac{1}{2}|(1-KB)^{-1}Q|^2\} \tag{3.10}$$

The usefulness of this identity depends upon an efficient algorithm for calculating $(1-KB(U))^{-1}Q$ since this needs to be calculated many times, in principle at every updating step. There are a number of different suggestions for this inversion problem of which the Gauss-Seidel is the method mainly used in applications (suggested by Weingarten and Petcher 1981). If $\chi$ is defined as $(1-KB(U))^{-1}Q$ then by rearranging we have

$$\chi = KB(U)\chi + Q \tag{3.11}$$

and this equation can be iterated until a satisfactory approximation to $\chi$ is found. This method has been implemented using the icosahedral subgroup of SU(2) on a $2^4$ lattice (Weingarten and Petcher 1981). Along similar lines, the method of Hamber (1981) proceeds by solving the same equation for $\chi$ by Gaussian iteration. In both versions the natural value of the initial vector in any iteration is the vector $\chi$ that resulted from the previous iteration. However, as with the previous method, the amount of computing time required to implement these algorithms on larger lattices is prohibitive.

The methods discussed above, although by no means exhaustive, give a picture of the difficulties faced in including fermions in lattice gauge field calculations and some of the ideas for overcoming them. Of the other methods for including fermions one that has been used successfully is that due to Hirsch, Scalapino and Sugar (1981) which is very efficient in two dimensions, although the difficulties

associated with generalizing it to higher dimensions have not yet been overcome. The method has also been applied to the Schwinger model (Martin and Otto 1982; Ranft and Schiller 1983). The microcanonical ensemble formulation of lattice gauge theory (Callaway and Rahman 1982,1983) also allows for the introduction of fermions in a natural way and is immediately amenable to parallel computing although the scheme has not yet been fully investigated, particularly in the fermionic sector. In the next section the pseudo-fermion method (Fucito, Marinari, Parisi and Rebbi 1981) will be examined and the methods discussed above serve as a yard-stick by which to measure its usefulness.

## 3.2 Pseudo-fermion methods

One of the undesirable features of a number of the fermionic techniques discussed in the previous section was that the amount of computer time required to update a link increased in proportion to the volume of the lattice, and thus severely limited the size of lattice that could be simulated. The reason for this was the essentially non-local character of the fermionic determinant, which couples all points in the lattice. In order to overcome this difficulty it is necessary to make some suitable approximation. The hopping parameter expansion is one such method, in which the higher order terms become increasingly non-local on the lattice. The pseudo-fermion method (Fucito, Marinari, Parisi and Rebbi 1981) which we will examine here is another such approximation. In this section we discuss three ways of implementing the pseudo-fermion approach: the Metropolis method and the Langevin method in both a first and

second order formalism. The essential feature of the pseudo-fermion method that makes it a viable computational scheme is that the amount of computer time required to implement it (beyond that required for a pure gauge simulation) is only increased by a factor N, independent of the size of the lattice. (N is the number of pseudo-fermionic iterations needed to achieve statistical equilibrium of the pseudo-fermions within some desired accuracy). Moreover the technique is ideally suited to implementation on a parallel or vector machine.

In a Monte Carlo simulation a new configuration $\{U'\}$ is generated from a previous one $\{U\}$, and if the change $\{\delta U\}$ is small, the expression (3.3) may be linearized:

$$\Delta S_{eff}(U) = \Delta S_G(U) - \frac{1}{2}\sum_{I,J} K^{-1}_{IJ}(U)\frac{\delta K_{JI}(U)}{\delta U}\delta U + O(\delta U)^2 \qquad (3.12)$$

Thus the problem becomes essentially one of finding the inverse matrix elements $K^{-1}(U)$ for sites neighbouring the link being updated. There are a number of standard techniques for such problems, some of which were discussed in the last chapter. The relaxation method, which involves the large time behaviour of the differential equation

$$\frac{dG_{IJ}(t)}{dt} = -K_{IL}(U)G_{LJ}(t) + \delta_{IJ} \qquad (3.13)$$

is one very general technique, of which the Gauss-Seidel iteration scheme is a special case. Another method that in general converges far more rapidly is the conjugate gradient method of Hestenes and Stiefel (1952). These techniques are widely used in the evaluation of propagators in a background field, of the type used to extract the

mass spectrum from a lattice gauge theory. However, as we saw in a different context previously, they are not very useful for the type of problem being considered here since they involve a large number of inverse matrix elements, which are not required in (3.12), and large storage.

In the pseudo-fermion technique the required Green function elements $K^{-1}$ of eq.(3.12) are evaluated approximately using a stochastic procedure with bosonic variables to estimate the functional identity

$$K^{-1}_{IJ}(U) = \langle \phi^*_I \phi_J \rangle = \frac{\int \mathcal{D}\phi^* \mathcal{D}\phi \, \phi^*_I \phi_J \exp(-S_{PF})}{\int \mathcal{D}\phi^* \mathcal{D}\phi \exp(-S_{PF})} \qquad (3.14)$$

where $S_{PF} = \sum_{M,N} \phi^*_M K_{MN} \phi_N$ is the action for the pseudo-fermionic variables $\phi$.

In the Metropolis version of the method (Fucito et al. 1981) the inverse matrix elements $K^{-1}$ are taken as the average (denoted by a bar) over N Monte Carlo updates of the $\phi$ variables, and they are evaluated for each new configuration of the gauge field U. Both fields are updated using the standard Metropolis method, but with different actions. The pseudo-fermion field is updated according to the action of (3.14) and the gauge field with the effective action:

$$S_{eff}(U) = S_G(U) - \frac{1}{2} \sum_{IJ} \overline{\phi^*_I \phi_J} \, K_{IK}(U) \qquad (3.15)$$

Thus the effect of the fermions may be included in computer time that is only proportional to N, and independent of the size of the lattice. The exact result, apart from errors proportional to $(\delta U)^2$, is obtained in the limit $N \to \infty$. The method depends entirely on the

value of N which is required to give reliable results and this is not known a priori. In the simulation of the Schwinger model by Marinari, Parisi and Rebbi (1981a) it was found that the values of N required to extrapolate to $N\to\infty$ were manageable (typically between 5 and 60 over a range of masses).

The Langevin technique (Parisi 1981; Fucito and Marinari 1981) involves finding the required elements of the Green function by iterating the Langevin equation. This idea originates in the work of De Dominicus (1975) in the context of critical phenomena and has been developed by Parisi and Sourlas (1979) and Parisi and Wu Yongshi (1981). To illustrate the general method we look at the operator for a free scalar field $(-\nabla^2+m^2)$ and find its propagator. We introduce a scalar field $\phi(x,t)$, with a "spurious" time dependence, which obeys the Langevin equation:

$$\dot{\phi}(x,t) \equiv \frac{d\phi(x,t)}{dt} = -(-\nabla^2+m^2)\phi(x,t) + \eta(x,t) \qquad (3.16)$$

where $\eta(x,t)$ is a noise term with $\langle \eta(x,t)\,\eta^*(x',t')\rangle = 2\,\delta^d(x-x')\,\delta(t-t')$ and the brackets $\langle\ \rangle$ indicate an average over the noise. The solution of eq.(3.16) for general $\eta$ is

$$\phi(x,t/\eta) = \phi_s(x,t) + \int d^dx'dt' G(x,t;x',t')\,\eta(x',t') \qquad (3.17)$$

where $\phi_s(x,t)$ is the solution of the homogeneous equation (the special solution) and $G(x,t;x',t')$ is the Green function of the equation defined by

$$\left[\frac{d}{dt} + (-\nabla^2 + m^2)\right]\begin{pmatrix}\phi_s(x,t)\\ G(x,t;x',t')\end{pmatrix} = \begin{pmatrix}0\\ \delta^d(x-x')\,\delta(t-t')\end{pmatrix} \tag{3.18}$$

With the initial conditions $\phi_s(x,0)=\phi_0(x)$ and $G(x,0;x',t')=0$ the solutions of these equations are

$$\phi_s(x,t) = \int \frac{d^dk}{(2\pi)^d}\, e^{ik\cdot x - (k^2+m^2)t}\,\tilde{\phi}_0(k)$$

$$G(x,t;x',t') = \int \frac{d^dk}{(2\pi)^d}\,\frac{d\omega}{2\pi}\, e^{i[k(x-x')+\omega(t-t')]}\,\frac{\{1-e^{-(k^2+m^2+i\omega)t}\}}{k^2+m^2+i\omega} \tag{3.19}$$

where $\phi_0(k)$ is the Fourier transform of $\phi_s(x,0)$ and we note that $\phi_s(x,t)\to 0$ as $t\to\infty$ (for $m\neq 0$). The averages over $\eta$ are given by

$$\langle\phi(x,t)\rangle = \phi_s(x,t) \xrightarrow[t\to\infty]{} 0$$

$$\langle\phi(x,t)\phi(y,t)\rangle = \phi_s(x,t)\phi_s(y,t) + 2\int d^dx'\,dt'\,G(x,t;x',t')G(y,t;x',t') \tag{3.20}$$

$$\xrightarrow[t\to\infty]{} \int \frac{d^dk}{(2\pi)^d}\,\frac{e^{ik\cdot(x-y)}}{k^2+m^2}$$

and we have thus recovered the propagator of the free scalar field. In the more general case of an interacting field where the operator to be inverted (which we denote by $\Delta$ ) is positive definite the same identities hold. Expanding in terms of eigenfunctions of the operator $\Delta\,\psi_\lambda(x)=\lambda\,\psi_\lambda(x)$ we have

$$\phi_s(x,t) = \sum_\lambda \psi_\lambda(x)\, e^{-\lambda t}\,\tilde{\phi}_0(\lambda)$$

$$G(x,t;x',t') = \sum_\lambda \int \frac{d\omega}{2\pi}\,\psi_\lambda(x)\,\psi_\lambda^*(x')\, e^{i\omega(t-t')}\,\frac{\{1-e^{-(\lambda+i\omega)t}\}}{\lambda+i\omega} \tag{3.21}$$

and it is straightforward to show that

$$\lim_{t\to\infty} \langle \phi(x,t)\phi^*(y,t)\rangle = G(x,y) \qquad (3.22)$$

where here G(x,y) is the propagator associated with $\Delta$.

The operator of interest to us is the lattice version of the Dirac operator, $\not{\partial}+m$ (which will depend upon how we choose to represent the lattice fermions). In order to find the Green function for the fermionic operator $(\not{\partial}+m)$ we require not just a single Langevin field $\phi$ but rather two such fields. We call this the Langevin method I and it proceeds by simultaneously iterating the two Langevin equations (Marinari, Parisi and Rebbi 1981b):

$$\dot{\phi}_1(x,t) = -(\not{\partial}+m)\phi_1(x,t) + \eta(x,t)$$
$$\dot{\phi}_2(x,t) = -(-\not{\partial}+m)\phi_2(x,t) + \eta(x,t) \qquad (3.23)$$

where $\not{\partial}$ is the covariant lattice derivative with gauge fields, and $\phi_1$, $\phi_2$ and $\eta$ are complex numbers that sit at every site of the lattice. For general $\eta$ the solutions to these equations take the form of eq.(3.17). Expanding in terms of eigenstates $\psi_\lambda(x)$ of $\not{\partial}$, with eigenvalues $i\lambda$, the explicit solutions are

$$\phi_1^s(x,t) = \sum_\lambda \psi_\lambda(x)\, e^{(-i\lambda-m)t}\, \tilde{\phi}_1(\lambda) \qquad (3.24)$$

$$G_1(x,t;x',t') = \sum_\lambda \int \frac{d\omega}{2\pi}\, \psi_\lambda(x)\,\psi_\lambda^*(x')\, \frac{\{1-e^{-(i\lambda+m+i\omega)t}\}}{i\lambda+m+i\omega}$$

where the $\tilde{\phi}_1(\lambda)$ are the coefficients of the expansion. The solution for $\phi_2$ is obtained by replacing $i\lambda$ by $-i\lambda$. The Green functions $G_1(x,y)$ and $G_2(x,y)$ of the operators $(\not{\partial}+m)$ and $(-\not{\partial}+m)$ are then simply given by

$$G_1(x,y) = \lim_{t\to\infty} \langle \phi_1(x,t)\phi_2^*(y,t)\rangle$$

$$G_2(x,y) = \lim_{t\to\infty} \langle \phi_2(x,t)\phi_1^*(y,t)\rangle \qquad (3.25)$$

and in the free field case the characteristic time of approach to equilibrium is of order 1/m. An alternative method, which we call the Langevin method II, proceeds by calculating the Green function $G_3(x,y)$ of the Hermitean operator $(-\not{\partial}^2+m^2)$

$$\dot{\phi}_3(x,t) = -(-\not{\partial}^2+m^2)\phi_3(x,t) + \eta(x,t) \qquad (3.26)$$

and the associated Green function is

$$G_3(x,y) = \lim_{t\to\infty} \langle \phi(x,t)\phi^*(y,t)\rangle \qquad (3.27)$$

which has a characteristic time of approach to equilibrium of order $1/m^2$.

It is instructive to compare these pseudo-fermion methods for evaluating the required matrix elements of $K^{-1}$ with the more standard methods such as conjugate gradient and relaxation mentioned earlier. Using the Langevin or Metropolis methods we can compute the Green function $G(x,y)$ for all x and y at the same time, while in comparable computer time the relaxation procedure gives only $G(x,0)$. However, the pseudo-fermion methods have associated with them statistical

errors whereas the relaxation method is essentially exact. Consequently, in order to measure G(x,y) in the region where G is large (i.e. when x is close to y) the pseudo-fermion methods are more suitable, and to compute G in the region where $|x-y|$ is large the relaxation method (or something similar) should be used. The first situation is the one we encounter in the effective action (3.12) whereas the second situation is found when computing the mass spectrum of the theory.

One quantity that we are interested in measuring is the expectation value of the fermion fields $\langle\bar{\psi}\psi\rangle$. This quantity is simply related to the pseudo-fermions of the Metropolis method by $\langle\bar{\psi}\psi\rangle=m\langle\phi^*\phi\rangle$ (with the lattice spacing a=1 throughout). For the Langevin method I the expectation value is given by

$$\langle\bar{\psi}\psi\rangle = \frac{1}{2}\left[G_1(0,0) + G_2(0,0)\right] \tag{3.28}$$

and for the Langevin II method the relation is simply $\langle\bar{\psi}\psi\rangle=mG_3(0,0)$.

In the next chapter we explain how the method was actually implemented and the results obtained. There is, however, one very important feature of the Langevin method I that severely limits its usefulness and will be discussed here. It is clear that for the Metropolis method and Langevin method II each individual element $\chi=\bar{\psi}\psi$ contributing to the average $\langle\chi\rangle=\langle\bar{\psi}\psi\rangle$ is positive, whereas this is not the case for the Langevin method I. In order to examine the fluctuations the expectation value of the quantity $\chi^2$ was measured for all three methods. The results, plotted in Figures 2 and 3, show clearly the very marked difference between the Langevin

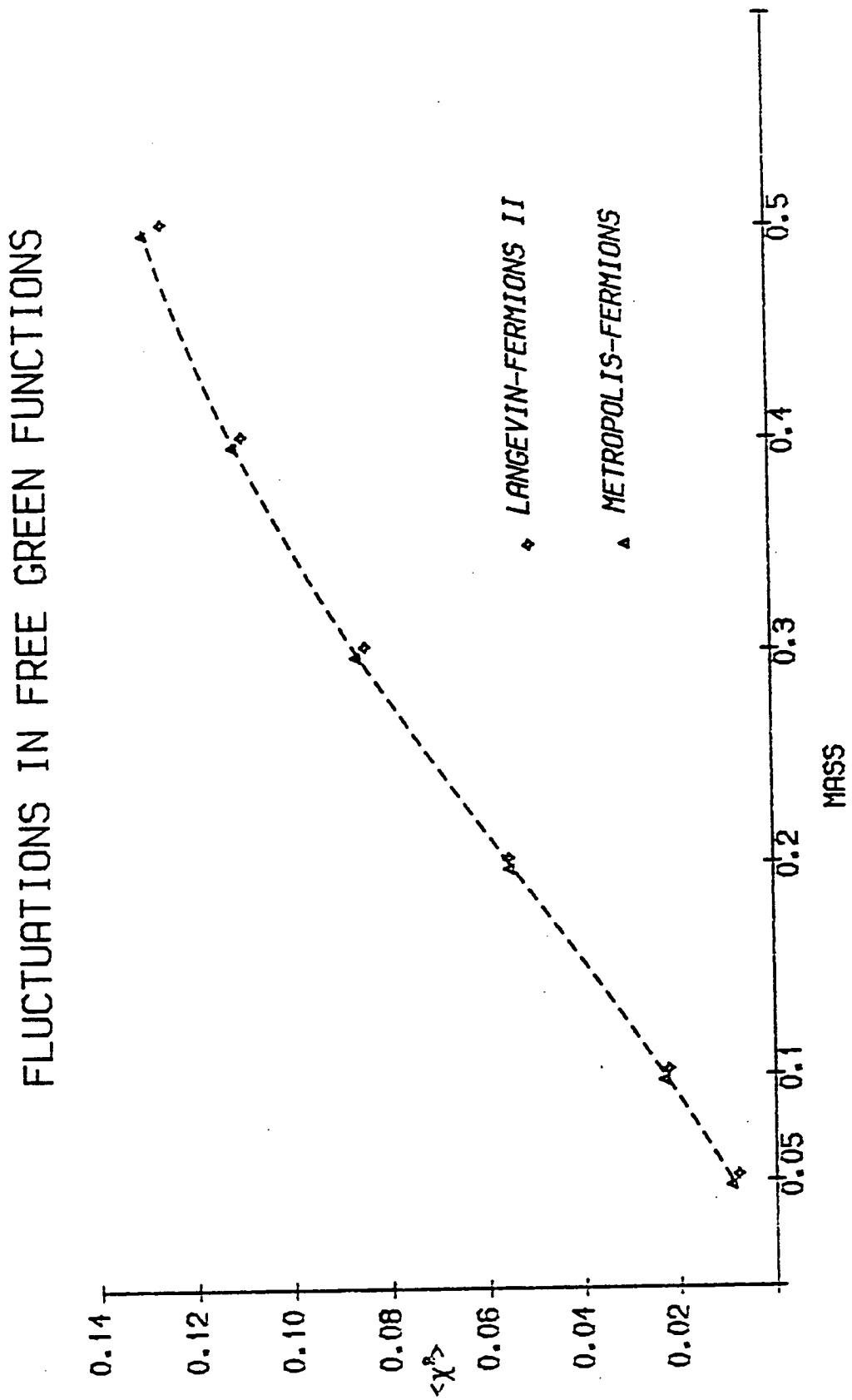



Figure 2 : The expectation value of the quantity $\chi^2$ is plotted for different masses using Metropolis and Langevin II fermionic techniques.

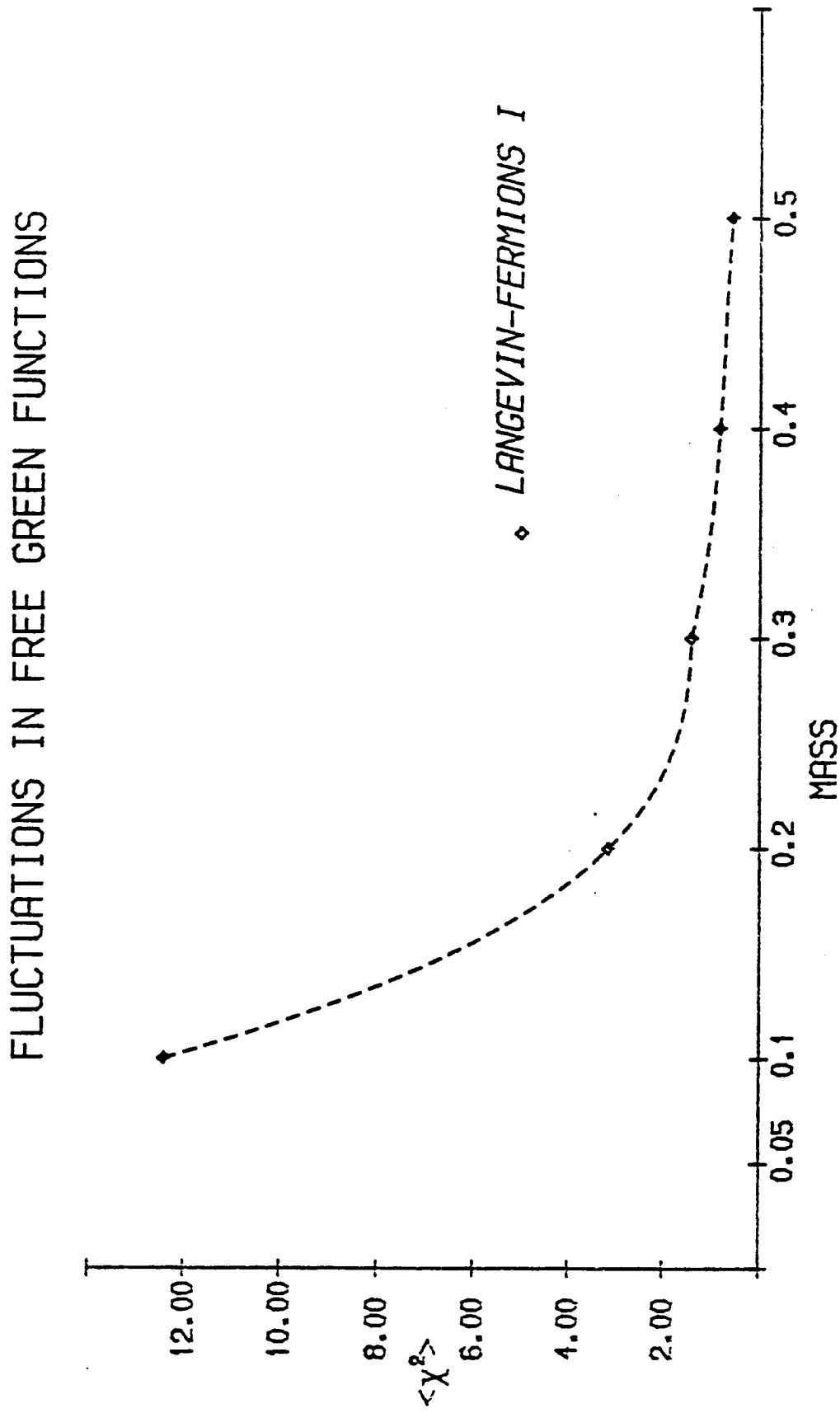



Figure 3 : The expectation value of the quantity $\chi^2$ is plotted for different masses using the Langevin method I.

method I and the other two methods. The observed divergence of $1/2m^2$ for the Langevin method I may be calculated analytically from the free-field versions of equations (3.23) to (3.25). In the expression $\langle \chi^2 \rangle$ for the Langevin method I there are terms $\langle \phi_1(x,t)\, \phi_1^*(x,t) \rangle$ and $\langle \phi_2(x,t)\, \phi_2^*(x,t) \rangle$ which, by carrying out the averages $\langle\ \rangle$ and completing the integration, may be shown to behave as $\sim 1/m^2$ for small masses. There is no such divergence in the calculation for the Langevin II method, where the fluctuations decrease as $m \to 0$ (see Figure 2). These large, indeed diverging, fluctuations arise from the fact that the operators in eq.(3.18) are not Hermitean. When interactions are present these fluctuations feed back into the gauge configurations giving spurious results, as we shall see. So although method I has a shorter time of approach to equilibrium in the region of small masses, where there is a critical slowing down, it proves not to be a useful method for implementing the pseudo-fermion technique.

Having established how the pseudo-fermion method may be implemented in practice we proceed to examine its usefulness in the context of the Schwinger model. In the next chapter we firstly outline the essential features of the Schwinger model, and particularly those aspects believed to be important in QCD. The Metropolis and Langevin methods are then compared in a simulation on a 64x64 lattice and some properties of the Schwinger model studied. We also examine the question of reducing the fermion doubling by decoupling heavy flavours.

In the past year a number of authors have looked at various aspects of the pseudo-fermion method. Otto and Randeria (1983) looked at the Schwinger model on a 4x12 lattice using Wilson fermions

and examined the limit $\delta U \to 0$ at $\beta = 2.5$ (corresponding to a correlation length of roughly one lattice unit). They concluded that the linear approximation (i.e. neglecting the order $(\delta U)^2$ terms) did not have a large effect on their measurements of the mass gap for a Metropolis hit size of 10% of $2\pi$. They also found that the correct results (by comparing with a Gauss-Seidel iteration scheme) were obtained in the extreme limit N=1, $\delta U \to 0$ showing that in this limit N does not necessarily need to be large, although the motion through phase space is very slow and a large amount of computer time is required as we would expect. Preliminary results have also been obtained in SU(3) (Hamber, Parisi, Marinari and Rebbi 1983) in which the quark condensate $\langle \bar{\psi} \psi \rangle$ and the average plaquette energy were measured. They also pointed out the possibility of using a heat bath algorithm for the pseudo-fermions rather than Metropolis and it is hoped that this will increase the convergence of the results and reduce the computer time required.

# CHAPTER 4

# TWO DIMENSIONAL QED

## 4.1 The Schwinger Model

The Schwinger model (Schwinger 1962) has proved to be an excellent testing ground for numerous ideas in field theory. The model is sufficiently simple to be amenable to analytic solution in various limits, but it also contains many of the features of interest in physical models. In particular it displays both the properties of asymptotic freedom and confinement, the former of which is known to be true in QCD and the latter is assumed to be so. These and other similarities lead one to hope that methods devised to investigate the Schwinger model may profitably be applied to QCD.

The theory describes a U(1) gauge field $A_\mu$ coupled to a fermion $\psi$ with mass m and charge g in two-dimensional space-time. The theory is both asymptotically free and confines the fundamental fermions (called quarks). The theory for massless fermions has an exact solution (Schwinger 1962; Lowenstein and Swieca 1971) while the massive theory is well understood (Casher, Kogut and Susskind 1974; Coleman, Jackiw and Susskind 1975; Coleman 1976).

The massive Schwinger model is defined by the Lagrangian density;

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi}(i\not{\partial} - g\not{A} - m)\psi \qquad (4.1)$$

where we use the notational conventions throughout:

$$x = (x^0, x^1) \quad , \quad \{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{4.2}$$

$$\bar{\psi} = \psi^\dagger \gamma_0 \quad , \quad \gamma_5 = \gamma_0 \gamma_1$$

The equations of motion are;

$$(i\partial\!\!\!/ - g A\!\!\!/)\psi = 0$$

$$j_\mu \equiv g\bar{\psi}\gamma_\mu\psi = \partial^\nu F_{\mu\nu} \tag{4.3}$$

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

The model is super-renormalizable by virtue of the fact that the coupling constant g has positive mass dimension;

$$[g] = [m] = (\text{length})^{-1} \tag{4.4}$$

This obviates the need for any infinite renormalizations, apart from a trivial renormalization of the zero-point energy, and as a result both g and m are finite (although bare) parameters. The dimensionless parameter that measures the interaction strength is m/g. When m/g goes to zero the model becomes the exactly soluble Schwinger model and when m/g goes to infinity the model becomes the exactly soluble free theory. Since the model is exactly soluble in both limits it is possible to do approximate calculations in both perturbation theory and strong coupling. Indeed, such calculations have been done and they will be discussed shortly. Firstly, however, we shall look at the exactly soluble massless model.

The spectrum of the theory may be derived from the boson representation (Bander 1976) where we make the replacement

$$\psi_{1,2}(x) = \left(\frac{\Lambda}{2\pi\gamma}\right)^{\frac{1}{2}} exp\left\{-i\sqrt{\pi}\int_{-\infty}^{x_1} dz\left[\pi(x^0,z) \pm \partial_1\phi(x^0,z)\right]\right\} \quad (4.5)$$

with $\Lambda$ a cutoff, $\gamma$ Euler's constant, and $\phi(x)$ a boson field with canonical momentum $\pi(x)$. For the massless theory the resulting action may be simplified to that of a massive boson field with $(mass)^2 \mu^2 = g^2/\pi$ and action

$$\pi(x)\partial_0\phi(x) - \frac{\pi^2(x)}{2} - \frac{(\partial_1\phi(x))^2}{2} - \frac{\mu^2}{2}\phi^2(x) \quad (4.6)$$

The solution of the massless theory exhibits what is believed to be a realistic mechanism of quark confinement via charge screening. This results from the strong polarizability of the vacuum and consequently the long range Coulomb force disappears. The above correspondence between the fermion and boson theory demonstrates explicitly that $\psi$ and all its excitations are absent from the physical space of states. All that remains is a free neutral pseudoscalar meson $\phi$ with mass $g/\sqrt{\pi}$ which can be thought of as a quark-antiquark bound state. This is an example of a dynamical Higgs phenomenon. Local electric charge conservation is spontaneously broken, but no Goldstone boson appears because the Goldstone mode may be gauged away. The solution also demonstrates a spontaneous breakdown of global chiral symmetry. This is associated with the appearance of an infinite family of degenerate vacuum states, labelled by an angle $\theta \in [-\pi, \pi]$ and global chiral transformations rotate one vacuum into another. Here again no Goldstone boson appears since the axial current is not conserved because of an anomaly (Jackiw 1973). Giving the fermions a mass changes the

Lagrangian of the boson field to

$$\frac{(\partial\phi)^2}{2} - \frac{\mu^2}{2}\phi^2 - \frac{m\Lambda}{\pi\gamma}\cos 2\sqrt{\pi}\,\phi \qquad (4.7)$$

The beauty of this approach is that the delicacies of normal-ordering become somewhat automatic.

This transformation from the fermion representation to the equivalent boson representation is a kind of duality transformation in that the roles of mass and coupling constant are interchanged. This makes (4.7) ideal for discussing the particle spectrum of the strongly-coupled Schwinger model.

Although the massive model is not exactly solvable it is possible to do perturbation theory in the mass parameter (Kogut and Susskind 1974; Coleman, Jackiw and Susskind 1975). One rather surprising observation is that the solution to the model involves the parameter $\theta$ which is totally independent of the coupling g and the mass m. The mass term, of course, explicitly breaks chiral invarience and removes the degeneracy of the vacuum. However, contrary to naive expectations, all the vacua remain stable as a result of the absence of Goldstone bosons. The field $\theta$ may be physically interpreted as the background electric field. Such a background field is not considered in standard treatments of four-dimensional QED, although it could be introduced. The reason is that such a field would have no effect, as it would be cancelled by pair production from the vacuum. However, the energetics of pair production in one spatial dimension are rather different and, in this model, give rise to different vacuum states. We only consider the case $\theta = 0$.

In a perturbative expansion with the mass as the perturbation

parameter the long range force between external charges of arbitrary magnitude does not disappear. From this it may be inferred that the Higgs mechanism does not occur. It may also be shown, independently of perturbation theory, that if the external charges are integral multiples of the fundamental charge g then the long-range force does disappear. This indicates that quark confinement takes place.

For $m<<g$ the theory describes a heavy pseudoscalar meson with weak self-interactions. Thus the theory always contains at least one particle: the original pseudoscalar meson of mass

$$M^{-}=g/\sqrt{\pi} + me^{\gamma} + O(m^2) \tag{4.8}$$

If it contains other particles they will be weakly-bound n-mesons, of mass $ng/\sqrt{\pi}$ (plus small corrections). In particular, the next particle is a scalar of mass

$$M^{+}=2M^{-} - \pi^2 e^{2\gamma} m^2/M^{-} + O(m^3) \tag{4.9}$$

When the mass of the fermion becomes infinite it decouples and the model reduces to a pure U(1) gauge theory which may be solved by transfer matrix techniques. Indeed, the lattice formulation of a pure U(1) gauge theory may, by a suitable choice of gauge, be shown to be equivalent to a set of one-dimensional XY spin models. The free energy is

$$F = \ln I_0(2\beta) - 2\beta \tag{4.10}$$

and the average plaquette energy, proportional to the energy density,

is

$$\langle 1-\cos\theta_{\mu\nu}\rangle = \tfrac{1}{2}E = -\tfrac{1}{2}\frac{\partial}{\partial\beta}F \tag{4.11}$$

where $\theta_{\mu\nu}$ is the (directed) sum of links around a plaquette and $\beta=1/4g^2$. From these equations one may derive strong coupling expansions. In this always- confining theory a square Wilson loop ($\Gamma$) of area A is given by

$$W(\Gamma) = \left[I_1(2\beta)/I_0(2\beta)\right]^A \tag{4.12}$$

and the string tension T is therefore

$$\begin{aligned} T &= \ln\left[I_0(2\beta)/I_1(2\beta)\right] \\ &= \ln\beta + O(\beta^2) \qquad (\beta << 1) \\ &= \frac{1}{4\beta} + O\left(\frac{1}{\beta^2}\right) \qquad (\beta >> 1) \end{aligned} \tag{4.13}$$

Strong coupling expansions, which are very similar to the high-temperature expansions used so profitably in statistical mechanics, provide a systematic and straightforward (at least in principle) calculational scheme. The expansion parameter is 1/ga (a being the lattice spacing) and, when this is small, the kinetic terms may be treated as a perturbation on the static terms (Banks et al. 1977). The strong coupling limit is confining and in order to extract continuum results it is necessary to extrapolate to the weak coupling regime, typically by the use of Padé approximants, and high orders in the expansion are needed to make confident continuum

predictions. In order for the extrapolation from strong coupling to weak coupling to be smooth it is necessary that there be no intermediate phase transition. This appears to be the case from both Monte-Carlo simulations of the pure gauge system and approximate renormalization group calculations (Migdal 1975; Kadanoff 1976), which seem to indicate that four is the lower critical dimension for gauge systems.

These methods have been applied to QCD (Banks et al. 1977) and were found to give reasonable results to fourth order, with the exception that the pion, rather than having zero mass, was found to be nearly degenerate with the rho. Although the situation is expected to improve at higher orders such calculations are extremely complicated. These methods have also been applied extensively to the Schwinger model (Banks, Susskind and Kogut 1976; Carroll et al. 1976; Kenway and Hamer 1978) and provide generally good agreement where they can be compared with exact results, although there are problems for the two species model in extrapolating to the chirally symmetric massless limit from the non-symmetric strong coupling regime.

The behaviour of Wilson loops when massless fermions are coupled to the gauge theory has been studied recently by Baaquie (1982). The Wilson loop for a circular contour of radius L is

$$W = -\pi (gL)^2 I_1(mL) K_1(mL) \qquad (4.14)$$

where $I_1$ and $K_1$ are the associated Bessel functions of the first and second kind and $m^2=g^2/\pi$ . This expression for W is exact and is a monotonically decreasing function of L that has the asymptotic behaviour

$$\lim_{L\to\infty} W \sim \begin{cases} -L^2 & , \ g^2 = 0 \\ -L & , \ g^2 > 0 \end{cases} \tag{4.15}$$

This is consistent with the notion that the gauge field is responsible for the confinement of the quarks and that as we attempt to separate a quark-antiquark pair it eventually becomes energetically favourable for a new pair to materialize from the vacuum. This both shields the long-range force and produces not a separated quark and antiquark but rather two quark-antiquark bound states with the consequent change from area to perimeter law behaviour of the Wilson loop.

Baaquie (1982) also calculates the propagator for the gauge-invariant quark-antiquark state in the continuum massless theory and finds that

$$\langle \bar{\psi}(x)\psi(x)\bar{\psi}(0)\psi(0)\rangle \xrightarrow[x\to\infty]{} \frac{g^2}{8\pi^3} e^{2\gamma} \tag{4.16}$$

This indicates that chiral symmetry is broken for the vacuum state and the $\langle\bar{\psi}\psi\rangle$ expectation value is given by

$$\lim_{m\to 0} \langle \bar{\psi}\psi\rangle = \frac{g}{2\pi^{3/2}} e^{\gamma} \tag{4.17}$$

The SU(2) flavour Schwinger model, in which there are two massive Dirac particles, an 'up' (u) and a 'down' (d) quark, exhibits some new features. As in the case of the ordinary Schwinger model some exact results are known about the low-energy particle spectrum for both strong and weak coupling (Coleman 1976). Taking the two fermion

species u and d to have masses $m_u$ and $m_d$ and equal electric charges g, the Lagrangian of the theory is

$$\mathcal{L} = \bar{u}(i\not{\partial} - m_u - g\not{A})u + \bar{d}(i\not{\partial} - m_d - g\not{A})d - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \tag{4.18}$$

For $m_u=m_d=m$ the theory has an internal global SU(2) symmetry which we call isospin. As with the one-species model the theory is super-renormalizable and hence asymptotically free.

It is known (Coleman 1973) that in two dimensions there is no spontaneous breakdown of continuous internal symmetries, unless the current-conservation equations are afflicted with anomalies or the Higgs mechanism occurs. Since neither happens here the particles of the theory reside in isospin multiplets when $m_u=m_d$ and chiral symmetry is restored in the massless limit. As with the massive one-species Schwinger model the particle spectrum consists solely of mesons, which can be thought of as quark-antiquark pairs tied together with gauge strings of constant tension (the case $\theta=\pi$ requires special attention, but it does not concern us here). The lowest lying multiplet is an isotriplet of pseudoscalar mesons which can be identified with the 'pion'. For small m/g these low-lying particles respect isospin symmetry even when it is broken at the level of the quark masses (Coleman 1976). This is an interesting result that we have investigated using a Monte Carlo simulation of the two species lattice Schwinger model and which will be discussed later in this chapter. The next lightest particle in the theory is an isosinglet and the isosinglet/isotriplet mass ratio is $\sqrt{3}$ (whatever the value of $\theta$). If there are other stable particles in

the model, they must be $O([g/m]^{2/3})$ times heavier than these.

## 4.2 Simulation of Two Dimensional QED

The Schwinger model contains many of the features that are of interest in physical models and the theory may be solved exactly in certain limits, as discussed in the previous section. However, our interest here is not only in the Schwinger model but also in fermionic techniques in lattice gauge theory. What we wish to examine is the relative accuracy and speed of convergence of the algorithms in a theory that has a number of the properties believed to be important in QCD. In this section two pseudo-fermionic methods, the Metropolis and Langevin methods, are extensively discussed and their relative advantages and disadvantages examined (Burkitt 1983). In the next section we look at some of the properties of the Schwinger model in more detail, and particularly at the dependence of the chiral properties of the theory on the number of fermion flavours. The simulations were done on the ICL Distributed Array Processor (DAP) at both Queen Mary College and Edinburgh. The lattice size used for all the simulations was 64x64.

The computer architecture plays an important part in the formulation of any large scale computing problem. This is particularly so with a parallel processor such as the DAP. Indeed, the limitations of present day computers in terms of both speed and memory size is often the determining factor in the viability of any Monte Carlo scheme. It is precisely these limitations that immediately rule out even considering the direct use of Grassmann variables for fermions or the direct evaluation of the fermionic

determinant for any lattices of reasonable size in greater than two dimensions.

The reliability of our results presented here were checked by observing their stability with respect to longer runs, different starting configurations and different random numbers and also agreement of extrapolation (in the limit of vanishing quark mass) to an analytically known result. In order to make meaningful remarks about the speed and efficiency of any simulation some knowledge of the particular computer used (both hardware and software) is necessary. To this end an appendix has been included giving some details of the working of the DAP. This appendix serves as both a companion to the remainder of this chapter and also as an introduction to some of the computing ideas that are becoming increasingly important, particularly in the realm of large scale computing.

The effective action for the lattice Schwinger model is given by eq.(3.3), where K(U) is the lattice version of $-\not{\partial}^2+m^2$ and Kogut-Susskind fermions are used. In this simulation we attempted to reduce the fermion doubling by using the square root of the fermionic determinant in the effective action for the gauge field (Marinari et al. 1981, Hamber et al. 1983). In later work we demonstrated that this method for reducing the number of fermion flavours does not work in two dimensions and this will be discussed more fully in the next section. Although the actual numbers obtained for physical quantities are not reliable, particularly at low fermion masses, this does not effect our conclusions on the relative values of the various algorithims. Checks made using the two-species model (i.e. without the spurious square root) produced the same picture.

The overall scheme of the simulation was firstly to take a gauge field configuration in equilibrium at some particular value of the fermion-gauge field coupling g. This gauge field configuration was generated in the usual way using a Monte Carlo algorithm, as explained in the first chapter. This was particularly straightforward in the case of the Schwinger model since the two dimensional U(1) gauge field can be simply parameterized by an angular variable $\theta(n)$ at every site n of the lattice. The value $g^2=1/3$ in lattice units was used throughout in order to ensure that the lattice of 64x64 was big enough in laboratory units to adequately describe the continuum physics. Using the exact Schwinger model result this corresponds to a correlation length of approximately four lattice units. Finite size effects only become significant for $m_u < 0.03$ on a lattice of this size, permitting a fairly unambiguous extrapolation to zero quark mass. The fermions were then introduced and allowed to equilibrate w.r.t. the gauge field. Finally the gauge field was updated according to the Metropolis algorithm with the effective action. New trial values of the gauge field variables were chosen in the range $\pm 0.1$ radians of the existing value. This value of $\pm 0.1$ was a compromise between the small errors of order $(\delta U)^2$, introduced by the linearization of the term $\delta[\mathrm{Tr}\ell n K(U)]$, and the longer correlations between successive gauge field configurations introduced by smaller angles of update. Smaller angles of update would give a slower motion through phase space and require a consequent increase in computer time to produce reliable results. After each update of the entire gauge field the required inverse propagators were calculated using one of the fermionic techniques, and the value obtained was fed back into the next evaluation of the

effective action for the subsequent update of the entire gauge field. In this way the simulation continued to generate configurations with the Boltzmann probability distribution as determined not just by $S_G(U)$, the pure gauge part of the action, but by $S_{eff}(U)$, to which the effect of fermionic loops contribute. Measurements are then made in the standard way by averaging over successive Monte Carlo configurations.

In order to measure how close or far from equilibrium the system was we measured the chiral symmetry breaking expectation value $\langle\bar{\psi}\psi\rangle$ (as in Marinari et al. 1981), and the average plaquette energy $W=\langle 1-\mathrm{Tr}U_p\rangle$, where $U_p$ is the product of link variables U around a plaquette. Since it is ultimately quarks of low masses that are of interest in QCD, it is the massless limit of these quantities that we wish to examine.

In our calculation using the Metropolis pseudo-fermions the expressions (3.12) and (3.14) were actually implemented in a more efficient way using the identity

$$\Delta S_{eff}(U) = \Delta S_g(U) - \frac{1}{4}\mathrm{Tr}\,\Delta\not{\partial}[(\not{\partial}+m)^{-1} - (-\not{\partial}+m)^{-1}] + O(\delta U)^2 \qquad (4.19)$$

where the inverse matrix elements (in square brackets) are calculated using

$$(-D+m)^{-1}_{IJ} = \frac{1}{Z_{PF}} \int \mathcal{D}\phi^* \mathcal{D}\phi \; \phi^*_J [(\not{\partial}+m)\phi]_I \exp(-S_{PF}) \qquad (4.20)$$

where $Z_{PF}$ is the Partition function for the pseudo-fermionic variables, and there is a similar expression for $(\not{\partial}+m)^{-1}$. This method has the advantage that all covariant derivatives are first

order and at no stage must $\not{D}^2\phi$ be calculated directly. This was of considerable practical importance since, in general, the calculation of $\not{D}$ acting on a variable is the most time consuming part of any such simulation. Only the values of $\phi$ and $\not{D}\phi$ needed to be stored at every site of the lattice. In the updating of the pseudo-fermionic variables it was found that the optimal interval (i.e. roughly half the variables updated) for choosing new values was approximately $\pm 1.2$, which was true for the whole range of quark masses and was broadly the same as for the simulation without the gauge field. It would appear that there are two important "time" scales for the pseudo-fermionic Monte Carlo; the number N1 of updates before taking any values for averaging (i.e. for equilibration), and the number N2 of updates which are averaged over to obtain the required Green function elements. However, it was found that the results were almost entirely independent of N1, and dependent upon N2. This is unsurprising since in any single update of the gauge field the gauge field variables change by very little, whereas the pseudo-fermionic variables may change quite substantially in a single update. The pseudo-fermionic variables are, of course, stored between successive gauge field updates. Thus it was found unnecessary to include N1 at all. As the fermion mass decreased a critical slowing down of the convergence of the algorithm was again observed (Marinari et al. 1981), in keeping with the fact that the Gaussian integrals that we are approximating become broader, and thus require more Monte Carlo hits to obtain a reasonable accuracy. In principle the exact result is obtained in the limit $N2 \to \infty$. Figure 4 shows the measurements of $\langle \bar{\psi}\psi \rangle$ at various values of the mass. The values plotted are those considered to be "optimal" in the sense that they are the values of

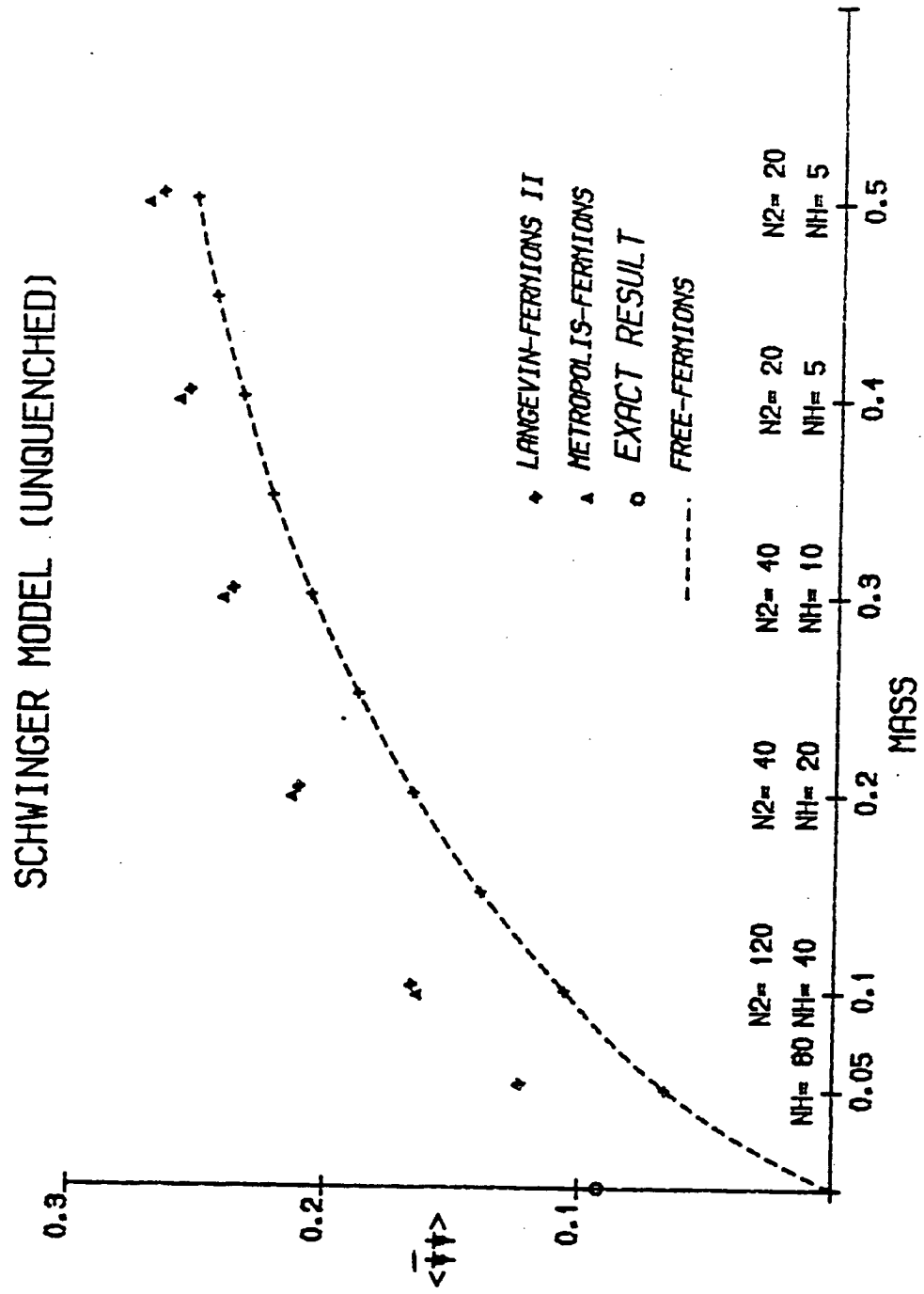



Figure 4 : The expectation value $\langle \bar{\psi}\psi \rangle$ plotted at various values of the fermion mass. The dashed line indicates the analytic result for free fermions on an infinite lattice. The points represent measurements for the Unquenched Schwinger model on a 64x64 lattice at the masses given on the horizontal axis. Optimum values of N2, the number of updates for the Metropolis method, and NH, the number of iterations of the Langevin equation, at various values of the mass are given.

N2 (given on the horizontal axis) at which the technique converges reasonably well (to within 3%). i.e. Increasing N2 above these values does not significantly increase the accuracy of the measurements. Figure 5 shows the actual approach of $\langle\bar{\psi}\psi\rangle$ to some fixed value as N2 increases (the horizontal axis) at a quark mass of 0.1 (in lattice units).

In implementing the Langevin method there are also two "time" scales: the time $\tau_1$ required for the pseudo-fermionic variables to equilibrate after an update of the gauge field and the time $\tau_2$ over which the average of random fluctuations $\langle\eta\eta^*\rangle$ is evaluated. It was found that $\tau_1$ was the time scale controlling the convergence of the method, and that the results for different values of $\tau_2$ were indistinguishable within the statistical error of the measurements. Thus, at each value of the mass in Figure 4 only the optimal value of NH is given, where NH=$\tau_1$/(step size (0.1)). A step size of H = 0.1 was used throughout in the Runge-Kutta discretization of the "time" evolution of the Langevin equation, thus ensuring that the errors due to the discretization remain small (they are of order $H^2$). The approach to some stable value of $\langle\bar{\psi}\psi\rangle$ at a quark mass of 0.1 is shown in Figure 5, where the horizontal axis labels the number of time steps, NH.

In order to compare the two methods we must not only give the times taken for an update/iteration but also some relevant information of how the calculation was carried out on the DAP (see appendix) and particularly how this would affect an unquenched simulation of QCD. In the Metropolis technique one is restricted by the requirements of detailed balance whereby all sites on a lattice may <u>not</u> be updated simultaneously, unlike an iterative procedure

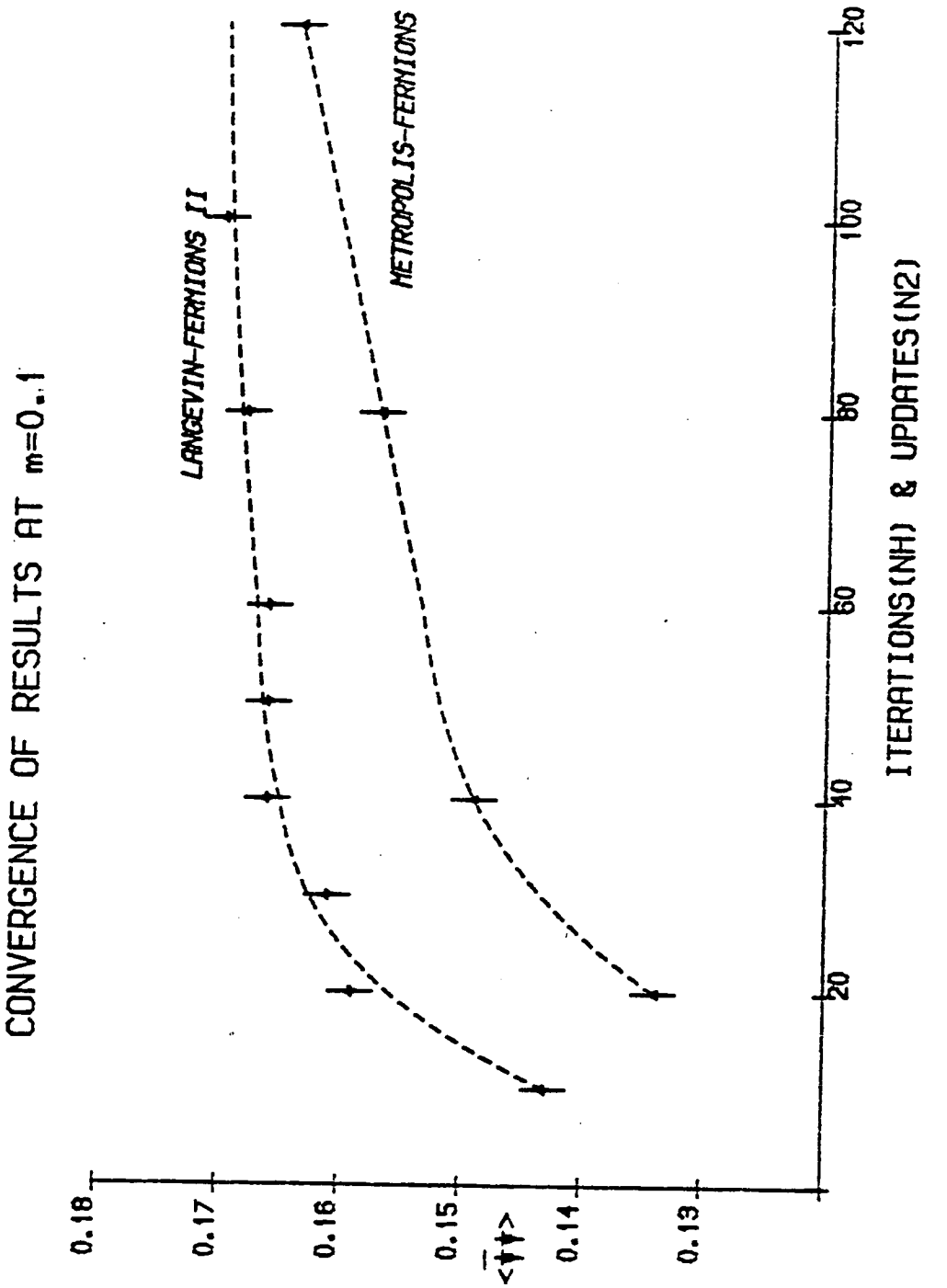



Figure 5 : Plot shows the convergence of the results of the measurement of $\langle \bar{\psi}\psi \rangle$ for Langevin method II and Metropolis method at m=0.1 as the number of iterations (NH) and updates (N2) are increased (resp.).

where all the sites may be treated simultaneously. In the simulations discussed here each site of the lattice corresponded to one processing element of the DAP and, as a result, the efficiency was reduced by a factor of four in the Metropolis pseudo-fermion technique. It is worth pointing out that in an unquenched QCD simulation this is unlikely to be a problem since we may distribute the calculation in such a way that, although a particular site is not being updated (on grounds of detailed balance) it is used for evaluating part of the update calculation for a nearby site that is being considered for updating. In a U(1) gauge theory like the Schwinger model this procedure would not produce any significant increase in efficiency since the gauge variables are simple angles, but for theories like QCD with a more complicated gauge group this procedure could result in considerable savings of computer time. For the calculations presented here the time taken for a single complete Metropolis pseudo-fermion update of the lattice was 0.16 sec, and for a single iteration of the Langevin equation was 0.13 sec. Thus, it is clear from Figures 4 and 5 that the Langevin technique is the faster of the two techniques in the way in which they were implemented in this simulation.

The Langevin method I, although fast to implement (the time taken for a single iteration of the lattice was 0.10 sec), gave spurious measurements as a result of the fluctuations mentioned earlier (see chapter 3 section 2). These large fluctuations feed back into the gauge field in the unquenched simulation and tend to increase the entropy of the system. As a result the value of $W = \langle 1-\mathrm{Tr}U_p \rangle$ increased above its free field value as the mass decreased - in contradiction to the results obtained from the strong coupling

expansion and using the other two pseudo-fermionic methods. Also the value of $\langle \bar{\psi}\psi \rangle$ was considerably larger than for the other two methods.

Thus we conclude that the Langevin method II is an efficient way of implementing the pseudo-fermionic technique in the Schwinger model. This result, however, is a particular feature of both the Schwinger model (being a U(1) gauge theory) and the DAP and is unlikely to be the case for QCD where the Metropolis method would appear to be superior for the reasons outlined above. A further improvement to the pseudo-fermion method may be obtained by using a heat bath (Hamber et al. 1983) rather than a Metropolis algorithm. Experience with the heat bath method in quenched gauge field calculations (Bowler and Pendleton 1983) seems to suggest that it produces a more rapid convergence. Moreover, the Gaussian nature of the pseudo-fermionic action ensures that the method is quite straightforward to implement.

## 4.3 Flavour Decoupling

The correspondence between Susskind and Dirac-Kahler fermions (Becher 1981; Becher and Joos 1982a,b; Rabin 1982; Banks et al. 1982) that we developed in chapter 2 enables us to interpret the $2^{d/2}$ degeneracy of Susskind fermions as a flavour degeneracy (Burkitt, Kenway and Kenway 1983; Mitra 1983; Kluberg-Stern et al. 1983; Becher and Joos 1982b). This identification was extended to enable us to give different masses to the different flavours and it will be recalled that in the Susskind formulation mass terms which are equivalent in the continuum limit of the theory will look different

on the lattice. This is possible since the lattice identification of flavours is ambiguous up to terms which are irrelevant in the continuum limit. In particular, the most suitable mass term for numerical simulations is the one which is most local on the lattice. We have shown that in two dimensions this corresponds to a one-link operator, which is no more non-local than the derivative term. In four dimensions where there is a fourfold degeneracy it is necessary to introduce one-, two- and three-link operators to completely break the degeneracy. However, in order to do a numerical simulation of QCD a good first approximation is obtained by simply introducing a one-link operator to break the SU(4) flavour degeneracy to SU(2) isospin. This is done by setting $m_1=m_2<<m_3=m_4$ (in the notation of chapter 2 section 3) and identifying $m_1$ as the mass of the up (u) and down (d) quarks and $m_3$ as the mass of the strange (s) and charm (c) quarks. To investigate the low energy behaviour of QCD the mass $m_3$ may be made as large as possible for the s and c quarks to effectively decouple from the theory, although in practice the largest possible mass value is the cutoff $a^{-1}$ and the smallest is (lattice dimension)$^{-1}$ so that the ratio $m_{u,d}/m_{s,c}$ can be only of order $L^{-1}$ (on a lattice of $L^4$) whereas in the real world $m_u/m_s \sim 1/40$.

In this section we examine this possibility of giving the quark flavours different masses in the context of the Schwinger model (Burkitt and Kenway 1983). Using Susskind fermions with the usual local mass term $m\bar{\psi}\psi$ we expect to reproduce the results for the SU(2) flavour symmetric Schwinger model. The expectation values $\langle\bar{u}u\rangle$ and $\langle\bar{d}d\rangle$ were calculated as functions of the fermion masses, and the results were extrapolated to zero mass. For degenerate flavours we found that our results for $(\langle\bar{u}u\rangle+\langle\bar{d}d\rangle)/2$ were consistent with zero in

the massless limit in accordance with expectations for the SU(2) flavour Schwinger model (Coleman 1976). The results for the one-flavour model were reproduced by introducing a one link mass term and setting the mass of one of the quark flavours (the d quark) equal to the inverse lattice spacing. The d quark then decoupled from the gauge field and the one species Schwinger model remained. The expectation value $\langle\bar{u}u\rangle$ was measured as a function of the u-mass (with the d-mass held fixed at 1 in lattice units) and it was observed to extrapolate to the exact 1-flavour Schwinger model result in the massless limit (Schwinger 1962), indicating that the heavy flavour decouples from the continuum physics. We also tested the suggestion that the effect of one flavour may be removed by using the square root of the fermionic determinant in the effective action for the gauge field i.e. by including only half the fermionic contribution to the effective action (Marinari, Parisi, and Rebbi 1981; Hamber, Marinari, Parisi and Rebbi 1983). In this case we found that $(\langle\bar{u}u\rangle+\langle\bar{d}d\rangle)/2$ closely follows the result for 2 degenerate flavours and appears to extrapolate to zero in the limit of vanishing fermion mass, showing that the method fails in this instance. The prediction of Coleman (1976) that isospin symmetry is unbroken in the SU(2) Schwinger model for small quark masses was also addressed and the results support this proposition.

As before, the simulations were carried out on a 64x64 lattice using the pseudo-fermion method as described in the previous section. Because of the rapid variation of eq.(2.39) and eq.(2.40) for small $m_u$, we subtracted the appropriate free fermion result from that for the gauge theory, as suggested by Marinari et al. (1981) before attempting the extrapolation to zero mass. The value of the

gauge-fermion field coupling was chosen to be $g^2=1/3$ in lattice units (as in the previous section) so that the lattice was large enough to describe the continuum physics.

To study the light quark properties of the one- and two-species Schwinger models, and also the theory with the square root of the fermionic determinant, we started with a pure gauge field configuration and a free pseudo-fermion field at $m_u=m_d=1.0$. Successive simulations were done at light quark masses $m_u$ of 0.8,0.6,0.4 and 0.2 for each of the three cases. As $m_u$ was successively decreased the end configurations of both the gauge field and the pseudo-fermion field were used as the starting configurations for the following simulation. At each mass value 100 gauge field sweeps, using the Metropolis algorithm, were done, with 60 pseudo-fermionic sweeps at each gauge field update using the same values for the update angles of the gauge and pseudo-fermion fields as previously.

The light quark mass was then decreased from 0.2, as plotted in Figure 6, and the number of pseudo-fermionic updates per gauge field update correspondingly increased; typically from 60 to 200. The non-degenerate case required somewhat more pseudo-fermionic updates in order to equilibrate, from 60 at $m_u=0.2$ to 180 at $m_u=0.05$, whereas the degenerate cases both appeared to equilibrate at $m_u=0.05$ with 120 or 140 pseudo-fermionic updates. This was probably due to the extra non-locality of eq.(2.40).

In order to check the stability of the results longer runs with more pseudo-fermionic updates per gauge field sweep were done and, in addition, the light quark mass was wound back up from 0.04 to 0.15, again using consecutive configurations, in all 3 cases. The error

bars are an estimate of the statistical error obtained by averaging over a number of independent runs (i.e. from different starting configurations). Figure 6 shows clearly that the results for the one-species model are consistent with the exact massless continuum value of $\langle\bar{u}u\rangle$. This indicates that the unwanted fermion may be decoupled by giving it a mass of order the cutoff, with only a minor increase in computer time. The two-species results also clearly indicate the expected restoration of chiral symmetry in the massless continuum theory. The intermediate points are the measurements for the system with half the fermionic contribution to the effective action. It is clear that the values in this case are not consistent with the one-species massless continuum theory. Thus we are drawn to the conclusion that halving the contribution of the fermionic determinant to the effective action fails to describe the 1-flavour model for fermion masses less than 0.1 (in lattice units) in this two dimensional model. This could not be observed by Marinari et al. (1981) because the small size of their lattice prevented them from running at such small masses. One reason for this failure may be non-factorization of the fermionic determinant in the continuum limit due to the generation of a four-fermion interaction (which is renormalizable in two-dimensions). A series of runs were also done at $g^2=1/8$ and a light quark mass of $m_u=0.05$. This corresponds to a smaller lattice spacing in laboratory units and the same picture emerged as also shown in Figure 6.

This decoupling was studied further by calculating $\langle\bar{u}u\rangle$ and $\langle\bar{d}d\rangle$ for values of the mass ratio, $m_d/m_u$, in the range 1 to 20 holding $m_u$ fixed at 0.05, as shown in Figure 7. Three distinct regions were observed. For $1<m_d/m_u<2$ our results are consistant with unbroken

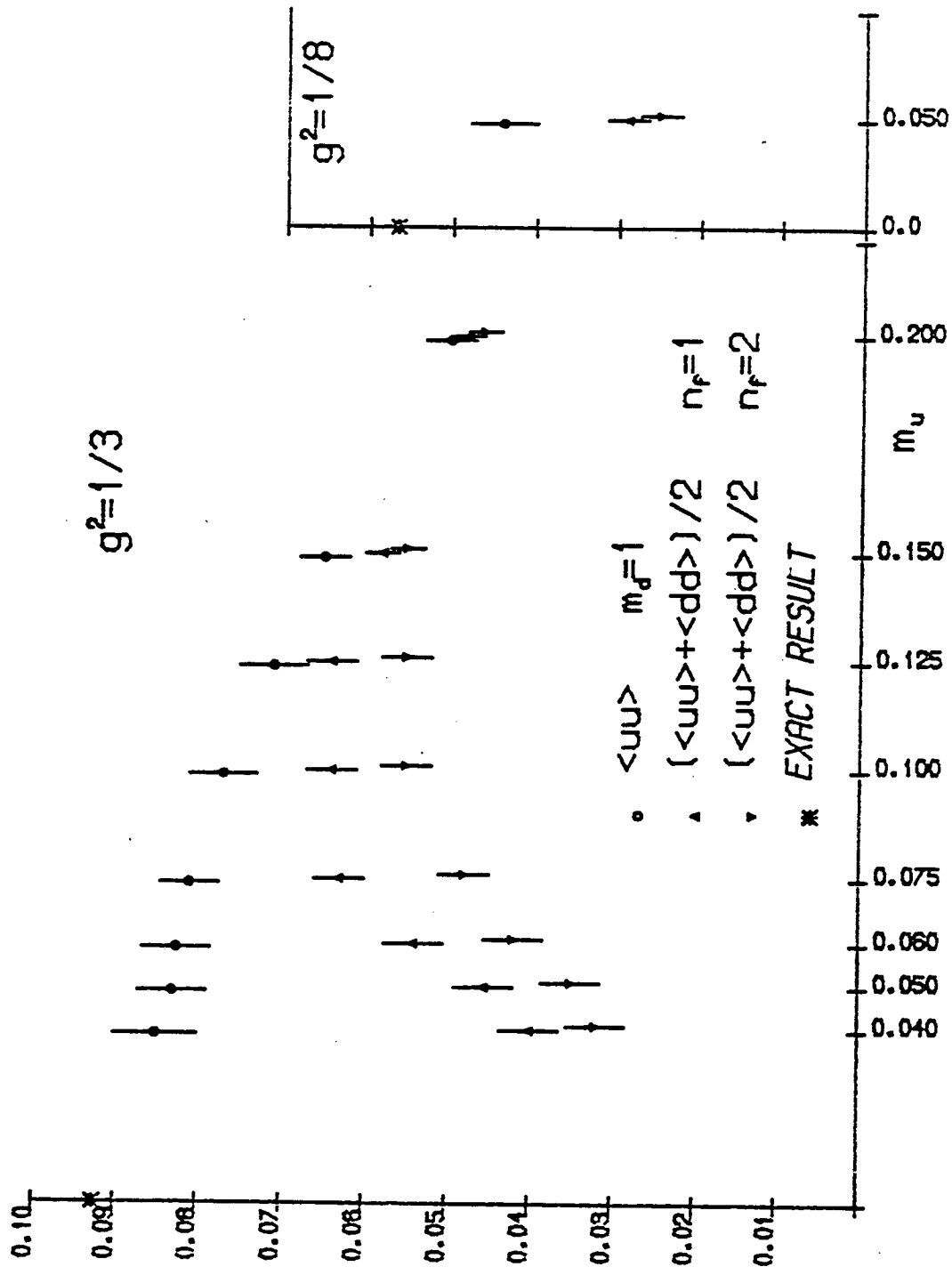



Figure 6 : Monte Carlo results for QED of 2 flavours on 64x64 lattice. Free fermion results have been subtracted out and n would be the number of flavours if the determinant factorized.

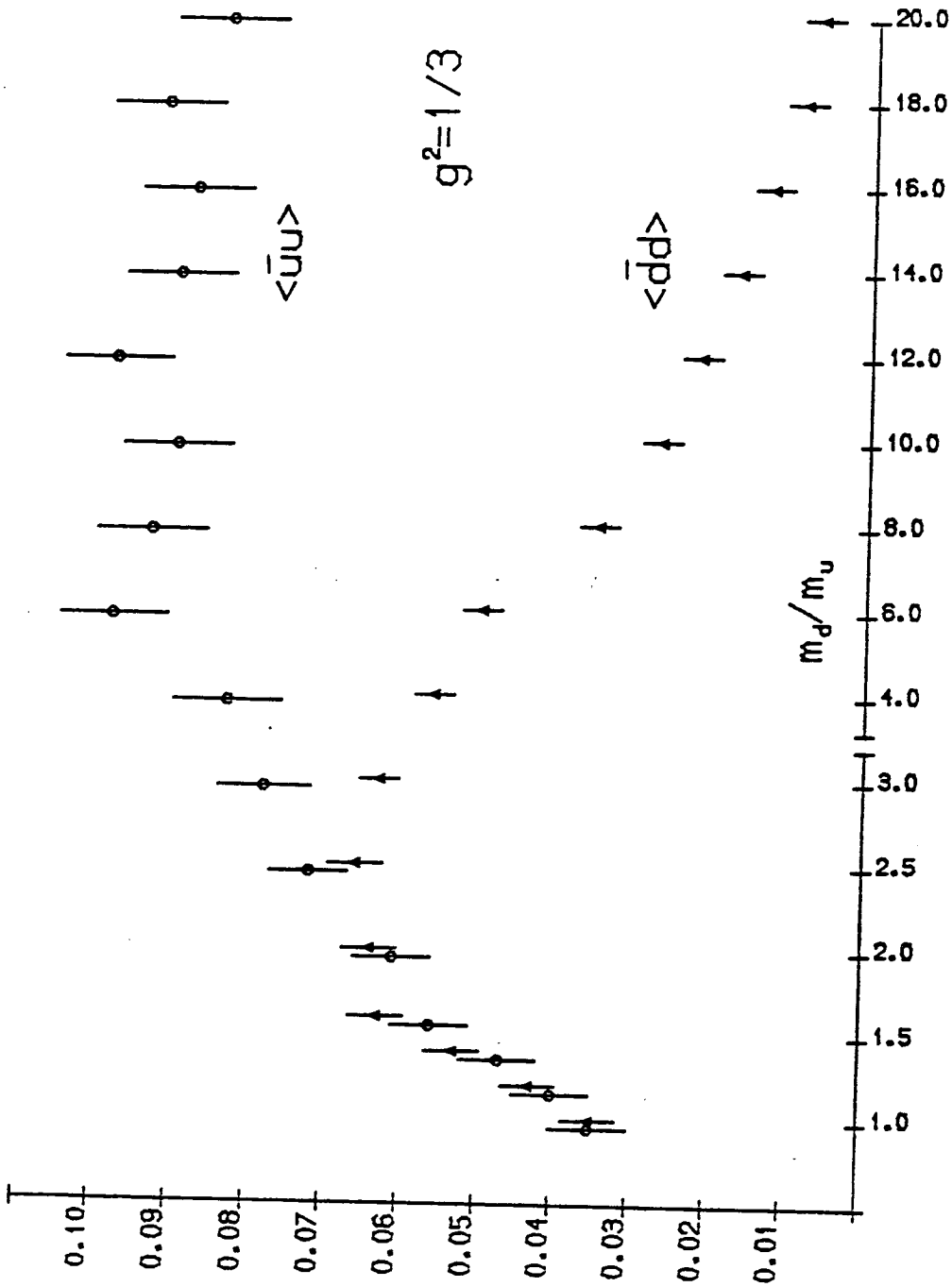



Figure 7 : Transition between 2-flavour and 1-flavour models as $m_u/m_d$ increases at $m_u$=0.05 and g=1/3.

isospin symmetry as suggested by Coleman (1976). For $m_d/m_u>10$ the flavours appear to have completely decoupled into a light fermion (u) interacting with the gauge field and a free heavy fermion (d). At intermediate mass ratios there is a crossover region. The actual transition between 1 and 2-flavour physics appears to be quite sharp, occurring at about $m_d/m_u=2.5$. We noticed a tendency for the Monte Carlo algorithm to get trapped in a metastable state here. These results suggest that the 1 and 2 flavour models are well separated in the variable $m_d/m_u$.

The results indicate that the method we propose for splitting the flavour degeneracy of Susskind fermions produces numbers that are in good agreement with known analytic results in two dimensions. Unwanted flavours may be decoupled from the theory by setting their mass to be of the order of the lattice cutoff and the resulting system appears to provide a good description of the remaining flavours. The increase in computing time (beyond that used for the usual degenerate flavours) to implement this scheme is fairly small. Moreover this method appears to be sensitive to the differences between the one- and two-species models at small quark masses and we are able to check some of the properties of the system that have been predicted from perturbation theory.

With regard to implementing this method in QCD some problems remain. In particular the fermions are defined on cells of size $2^d$. One consequence of this is that some of the operators corresponding to particle states will be non-local (i.e. spread over a unit cell) and the statistical accuracy will probably be lower as a result of the fluctuations of the gauge field links (which are required in order to maintain the gauge invariance). Also, with the lattice

sizes used at present (i.e. roughly $8^3$x16 or $10^3$x20) it is only possible to determine particle masses over a region of 8 to 10 lattice cells with this method and we thus have fewer points (compared with using Wilson fermions) from which to determine the masses using the exponential decay of the propagators. Nothing is known at present, however, about how the inclusion of dynamical fermions will affect the overall mass scale of a simulation or the resulting estimates of the absolute size of our QCD vacuum "box".

Furthermore, as pointed out in chapter 2 section 3, if a mass term is introduced to break SU(4) flavour symmetry to SU(2) there is no remnant of chiral symmetry on the lattice to prevent the u and d quarks from acquiring a mass. In fact the situation is completely analogous to Wilson fermions, and two renormalization conditions are required: one which fixes the pion mass to be zero (or its physical value) and one which fixes a strange meson mass to its physical value. Thus the two mass parameters $m_1$, $m_3$ must be tuned to fit the observed splitting between strange and nonstrange hadrons. It is an unfortunate fact that the only lattice theory with any remnant of chiral symmetry is SU(4) symmetric. On the other hand, our method has the advantage of being more economical (by a factor of four) in terms of computing time and memory requirements when compared with Wilson fermions since there is only one (complex) fermionic degree of freedom at every site.

## Conclusions

Lattice gauge theory has proved to be a fruitful way in which to study gauge theories. The lattice provides an explicit gauge

invariant regularization for the continuum field theory and enables us to carry out non-perturbative calculations. Confinement arises naturally in the strong coupling regime of lattice QCD and numerical results are consistent with the property of asymptotic freedom. The lack of any phase transition between the weak and strong coupling limits provides strong support to the proposition that asymptotic freedom and confinement are simultaneously properties of QCD. Moreover, there is the possibility of explicitly calculating the particle spectrum of the theory, and some significant progress in this direction has been made recently, although much remains to be done.

One of the fundamental problems in lattice gauge theory is the treatment of fermions. We have seen that the most straightforward transposition of the continuum description of fermions onto the lattice leads directly to the celebrated fermion doubling problem. A number of prescriptions for eliminating this doubling, even partially, have been proposed but all seem to have some undesirable features. The SLAC prescription eliminates the doubling entirely without breaking chiral symmetry but is very non-local on the lattice and gives non-covariant terms in the continuum limit of the theory. Wilsons' method also eliminates the doubling entirely by giving the unwanted fermions masses which are of order of the lattice cutoff.. However this method explicitly breaks chiral symmetry, although it is believed that the symmetry is restored in the continuum limit of the theory. This connection between doubling and chiral symmetry is a very deep one and has been shown to be intimately related to the topology of the lattice and the Adler-Bell-Jackiw anomaly. It places a very severe restriction on the theories which we can construct on

the lattice and, in particular, is a no-go theorem for putting the electro-weak theory on the lattice. Another scheme, due to Susskind, partially reduces the fermion degeneracy from $2^d$ to $2^{d/2}$ (in d dimensions) and chiral symmetry is manifested as a discrete translational symmetry of the theory.

Kahlers' geometric description of Dirac fermions is both an elegant and natural one in which to describe lattice fermions. The continuum and lattice versions of the Dirac-Kahler equation both have a $2^{d/2}$-fold degeneracy. In the continuum version this reduces to $2^{d/2}$ identical copies of the Dirac equation. However on the lattice the reduction to the lattice Dirac equation can only be done in momentum space. That the degeneracy of Dirac-Kahler and Susskind fermions on the lattice is the same is more than coincidence. The two descriptions are, in fact, equivalent in the case of free fields, although they interact differently with gauge fields. This equivalence enables us to explicitly identify the flavour degeneracy of the Susskind fermions. Although the flavours do not decouple on the lattice, it is possible to use the continuum identification and to break the degeneracy by introducing different mass terms for the different flavours. Since the lattice identification is ambiguous up to terms which are irrelevant in the continuum limit there are a number of equivalent mass terms which will look very different on the lattice. Consequently there exists a description which is optimal in the sense that it is the most local description that is possible on the lattice. We have found that this optimal description is simply a one-link operator in two dimensions while in four dimensions one-, two- and three-link operators are necessary to completely split the degeneracy. However, in QCD the low energy behaviour may be well

approximated by two degenerate light quarks (u and d) which can be described quite straightforwardly by introducing only a one link mass operator and giving the s and c quarks masses which are of the order of the lattice cutoff. The SU(2) symmetry that remains may be interpreted as isospin symmetry of the (degenerate) light quarks. This idea has been tested in the context of the Schwinger model where we find that the usual local mass term reproduces results consistant with the SU(2) Schwinger model. When a one-link mass term was introduced and one of the quarks decoupled by increasing its mass to the cutoff the results gave agreement with the one-species Schwinger model. Thus this method seems to be a viable way of eliminating the unwanted doubling in numerical simulations. One disadvantage of this approach is that the symmetries of the original Susskind formulation, which prevent the generation of mass terms in the fully interacting theory, are broken when we introduce the non-local mass term. Consequently the continuum limit of the theory must be identified in the same way as required with Wilson fermions by finding a critical bare mass of the light quark at which the pion mass vanishes (or some equivalent criterion). Also, since the fermions are defined on cells of size $2^d$, the operators corresponding to some of the particle states will be non-local. As a result the statistics of any such quantity will probably be worse than for local objects because of the fluctuations in the gauge field links. One significant advantage, especially from the computational point of view, is that this method requires only one fermionic variable on each site of the lattice, compared with four for Wilson fermions.

Establishing a consistent lattice definition of the number of continuum fermion species represents only one part of the whole

question of introducing fermions into lattice gauge theories. The other aspect concerns how fermions are to be introduced as dynamical variables that interact with the gauge field, rather than simply as static external sources. Solutions to this problem are only in the early stages of development and much remains to be understood. Until now almost all the results of lattice gauge theory have been obtained in the quenched approximation. However it is clearly of considerable importance that the degrees of freedom believed to be important in the real world are incorporated into the theory. After examining a number of proposals for introducing fermions we studied the pseudo-fermionic method in detail. Both the Metropolis and Langevin techniques for implementing the method were applied to the Schwinger model. By looking at the approach to equilibrium of the fermion expectation value over a range of masses it was found that the Langevin method was the faster of the two techniques. However, this result was very dependent upon the way the calculation was actually carried out on the Distributed Array Processor and is unlikely to be the case for simulations of QCD (even on the DAP). Furthermore, the Metropolis method may be considerably improved by using a heat bath algorithm and consequently it appears to be the most promising candidate for introducing dynamical fermions.

Recent work on extracting hadron masses from SU(3) lattice gauge theory indicates that the lattice sizes being used at present are too small to extract reliable numbers. The computer time and facilities required for these calculations is enormous. The viability of such calculations is intimately linked to the capabilities of the most modern computers and future developments in the field of computer technology will be one of the crucial factors in determining the type

and size of calculations that can be fruitfully done. It is becoming increasingly clear that one of the most significant advances for large scale simulations, especially in lattice gauge theory and statistical mechanics, is the appearence of parallel processing and vectoring machines. These machines, although only in the early stages of development at present, represent new and exciting prospects which it is to be hoped will continue to be developed. As a result, we are extremely fortunate to have been able to use a parallel processor for the calculations reported here. The methods we have investigated have all had the virtue that they could be implemented economically in parallel and it seems reasonable to assume that such considerations will become increasingly important for any practical calculational scheme in the future.

Because lattice gauge theory is already in the very forefront of large scale computing and since it would be prohibitively expensive at present to go to significantly larger lattices it is desirable to attempt to improve the Wilson action. In this way it would be possible to increase the physical size of currently used QCD lattices by going to stronger couplings g (and remaining in the scaling region). Preliminary results using two dimensional asymptotically free theories (Berg et al. 1983) are encouraging. At the same time improvements to the fermionic part of the action could also be considered, although this appears to be a more difficult problem. One practical argument in support of improved actions (in preference to calculating on yet larger lattices) is that dynamical fermion methods are more manageable (in terms of computing time required) on smaller lattices with improved actions rather than on larger lattices using the usual Wilson form of the action.

# APPENDIX

Calculations in lattice gauge theory lead naturally to a consideration of computer architecture. The viability of any simulation one may wish to perform depends foremost upon the computing resources available. Consequently the last decade has seen a flowering of interest by sections of the theoretical physics community in every aspect of computer technology (This has also been true of a number of other branches of both the physical and natural sciences). In this appendix we shall outline some of the features of the ICL Distributed Array Processor (DAP), which represents a new and important innovation in computer technology. The architecture of the DAP is discussed and two of the software features which are central in DAP calculations are explained. We look particularly at how the DAP is used in actual Monte Carlo simulations of lattice gauge theory. (see also Hockney and Jesshope 1981, Bowler 1983, and refs therein).

The DAP combines computational power with a technology that is inexpensive in a machine with a wide performance range. These two features combine to give the DAP an advantage over either the large and very expensive "supercomputers" such as CRAY, and purpose-built processors, which are inherently inflexible. Furthermore, the present versions of the DAP use only relatively modest technology and fairly low levels of integration. Developments in very large scale integration (VLSI) offer the prospect of substantial improvements in computational times and in the sizes of lattices that might be contemplated in lattice gauge theory simulations.

Architecture and Technology

The DAP is not a back-end processor but rather is designed to emulate a memory module for an ICL mainframe (called a host machine in this context). The DAP can provide memory to the host in the conventional way when it is not executing its own code, and data in the DAP store may be processed by either the DAP or the host computer. The basic hardware of the DAP, indicated highly schematically by Figure 8, consists of a 64x64 array (described as rows and columns) of processing elements (PE's), each having 4Kbits of memory (giving a total of 2Mbytes of memory attached to the host). The array is connected two-dimensionally, with each processing element having four neighbours to which it is connected. These are identified by the points of a compass N,S,E and W. The connections at the edge depend upon whether the machine is instructed to operate in planar or cyclic geometry. Planar geometry defines a zero input at the edges, whereas cyclic geometry identifies the ends of columns or rows. In addition to the 4Kbit store, each PE contains three 1-bit registers (labelled A,Q and C), two multiplexers and a 1-bit full adder, the most interesting of which is the A-register. Certain instructions may be made conditional upon the setting of the A-register in each processor. How this local autonomy may be exploited will be illustrated in the discussion of software features. There is also a master control unit (MCU) which handles certain simple scalar functions such as control of DO loop variables in Fortran, and which also broadcasts instructions to the processor array.

Software Features

To take advantage of the DAP's parallel processing power a language called DAP Fortran, which is based on Fortran, has been developed. A DAP program is run as a subroutine of a master Fortran program run on the host machine. Communication between the DAP Fortran and Fortran routines is achieved through the use of shared COMMON blocks, which are loaded into the DAP store. Processing is initiated in the usual way with control being passed to a Fortran master program which sets up the input routines and data, and might include some pre-processing to be performed by the host. Control is then passed to one of any number of DAP Fortran entry routines, which can in turn call other DAP Fortran routines. Periodically, or on termination of the run, control is passed back to the host for Fortran post-processing and output.

The three basic types of variables in DAP Fortran are scalars, vectors and matrices. A scalar corresponds to an ordinary Fortran variable whereas vectors have a range over 64 in a single dimension and matrices range over 64 in two dimensions. Variables and constants may be either of type REAL, of length 3 to 8 bytes, INTEGER, of length 1 to 8 bytes, or LOGICAL, and are declared in a similar manner to usual Fortran. For example, the code

```
DIMENSION A(,),B(,),C(,)          (A.1)
C=A+B
```

means that at every PE the value of A and B are added and put into the appropriate slot for C, and this is done simultaneously at each of the 4096 PE's.

The two DAP Fortran features which give it considerable flexibility involve the ability to shift information between PE's and

the use of logical matrices to provide local autonomy to the PE's. In order to bring information stored at one PE to another PE there are a number of shift operations. The operation of these shifts is best illustrated by an example:

```
DIMENSION A(,),B(,),C(,)                    (A.2)
C=B+SHWC(A,3)
```

The effect of this statement at any PE, which is illustrated in Figure 9, is to assign to C the sum of the element of B which is stored at that PE and the element of A which is stored three sites away in a easterly direction, with cyclic boundary conditions automatically imposed over all the 64 columns of PE's that run east-west. Similarly there are shifts north, south and east with either cyclic (SHNC, SHSC, SHEC) or planar (SHNP, SHSP, SHEP, SHWP) boundary conditions. It is also possible to use the DAP in long-vector mode, in which we may think of the numbers as being stored in a vector of length 4096. It is then possible to do shifts along this vector by means of the operations SHLC, SHRC, SHLP, SHRP which involve left or right shifts with either cyclic or planar boundary conditions at the ends of the vector.

Operations and assignments may be made conditional upon the value of logical matrices (called masks in this context) at the processing elements. The logical mask sets the A-register mentioned earlier. Such masks can be either generated within a program or defined using built-in logical functions available in DAP Fortran. e.g. the function ALTR(N) sets the first N rows .FALSE. and the next N rows .TRUE., and so on until completion. (Similarly ALTC(N) does the same with columns). More elaborate masks may be constructed using these standard logical operators in conjunction with both the shifts

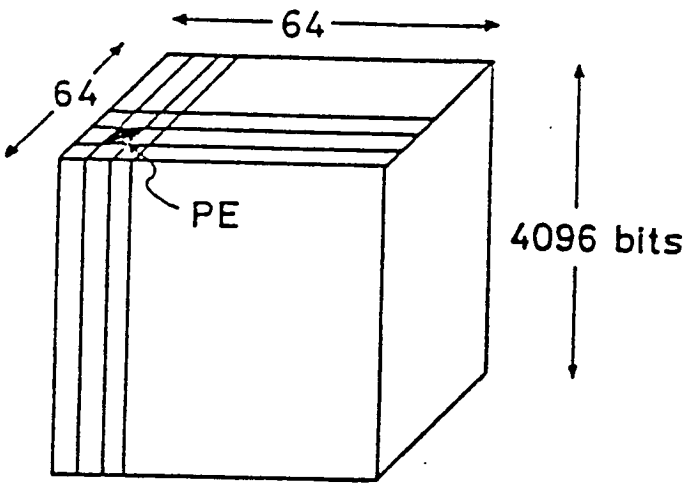



Fig.8

Figure 8 Highly schematic diagram of DAP hardware.

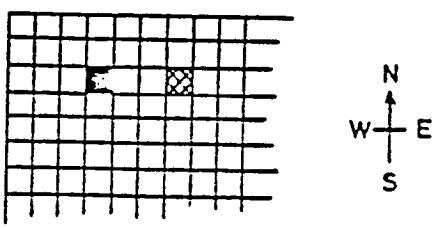



Fig.9

Figure 9 The effect of C=B+SHWC(A,3). The solid square denotes a typical PE, whilst the cross-hatched square denotes the location of the element of A accessed by the shift.

discussed above and standard logical statements. For example:

```
LOGICAL LMASK(,)                                    (A.3)
LMASK=ALTR(1).LEQ.ALTC(1)
```

sets up a chequerboard pattern in which each PE is alternatively .T. and .F., as illustrated in Figure 10. Assignments may then be made conditional upon such a mask in the following way:

```
REAL*4 A(,),B(,)                                    (A.4)
A(LMASK)=B
```

Only those elements of A at which LMASK is .T. are assigned the corresponding value of B, at all other PE's the value of A remains unchanged. Another important use of logical masks is in combination with the MERGE function:

```
DIMENSION A(,),B(,),C(,)                            (A.5)
C=MERGE(A,B,LMASK)
```

where LMASK is a LOGICAL matrix Here C takes the values of A at those PE's where LMASK is .T. and the values of B elsewhere.

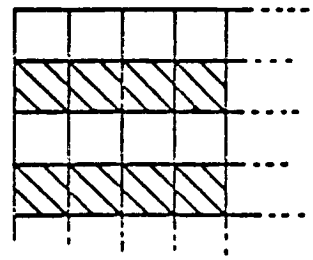
## Lattice Gauge Theory Calculations

The parallelism of the DAP makes it ideally suited to the Monte Carlo simulation of lattice systems in which essentially the same sequence of steps is repeated a large number of times. The question of how to use this parallelism in the most efficient way is an important one. The situation is very different from that with a serial computer, and we will discuss here some of the considerations that are important in the implementation of a lattice gauge theory simulation on the DAP. The first question is how to map the lattice variables onto the 64x64 DAP array. In the two-dimensional models considered in this thesis the straightforward identification of sites

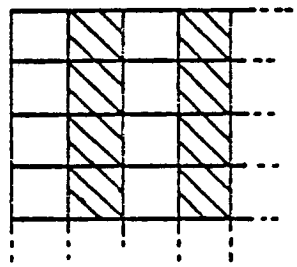
on the lattice with PE's was used and the natural choice of lattice size was 64x64. At each PE were stored the gauge fields which live on the links emanating in the positive direction from that site. In this way the locality of the action ensures that variables need only be moved between PE's that are near each other. However, in higher dimensions the situation becomes more complex. Here we will discuss the construction of an $8^4$ lattice on the DAP, although other sizes and/or dimensionalities of lattice are possible, and are discussed by Pawley and Thomas (1982). With an $8^4$ lattice there is again a one-to-one correspondence between sites of the lattice and PE's, although the actual distribution of sites over the 64x64 array requires care. There is a natural and elegant construction in which the 64x64 array is divided into 8x8 blocks of PE's, of which a portion is shown in Figure 11, and two of the four dimensions are mapped within the 8x8 blocks. The remaining two dimensions are mapped between blocks. Thus, the lattice neighbours of any PE are found one and eight away on the 64x64 array of PE's. The built-in cyclic boundary conditions of the DAP ensure the periodicity of the coordinates corresponding to the steps of eight PE's, but the periodic boundary conditions for the two coordinates which are mapped within each 8x8 block must be enforced explicitly. It is clear that the neighbours for the directions mapped into the 8x8 block will usually be only one away, except for those sites on the edge of the block. Consequently it is necessary to define neighbours explicitly, and this is most easily done by a combination of logical masks and MERGE operations. Consider, for example, sites on the eastern edge of the 8x8 blocks. Then the boundary mask, as indicated in Figure 12, defined by

(a)

LMASK = ALTR(1)



(b)



LMASK = ALTC(1)

(c)

LMASK =

ALTR(1).LEQ.ALTC(1)

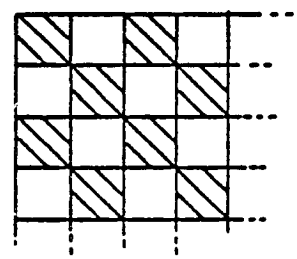


Figure 10 Logical masks on the DAP. The grid squares represent PE's.

(a) The effect of ALTR(1). Hatching denotes .T.

(b) The effect of ALTC(1).

(c) The effect of ALTR(1).LEQ.ALTC(1).

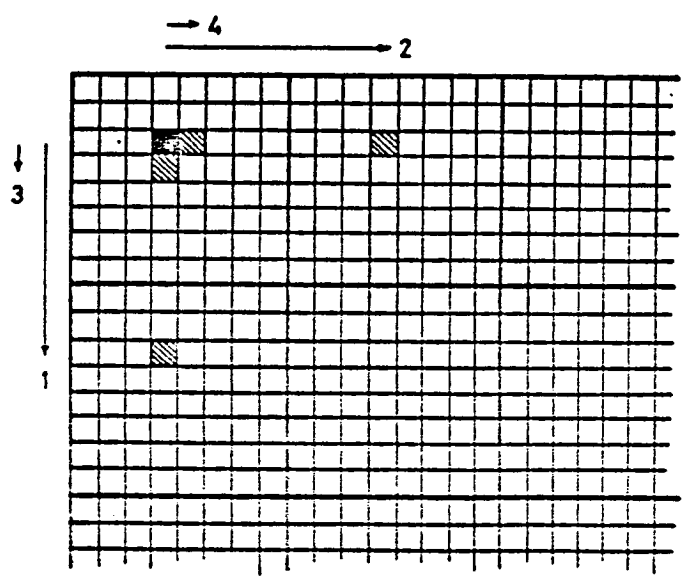



Figure 11 Mapping an $8^4$ lattice on to the DAP; nearest neighbours of a 'typical' site are located at the PE's shown.

```
LE=ALTC(8).LEQ.SHWC(ALTC(8),1)                    (A.6)
```

is .F. only at such sites. Neighbours in the easterly direction on the 8x8 blocks may then be defined by the statement

```
B(,)=MERGE(SHWC(A(,),1),SHEC(A(,),1),LE)          (A.7)
```

This has the effect of assigning to the array B the value of the array A stored at the next PE in the easterly direction if LE is .T. (i.e. for all PE's not on the easterly edge of an 8x8 block) and to assign the value of A at the PE seven away in the westerly direction for those PE's at which LE is .F. (i.e. those PE's on the easterly edge of an 8x8 block). This procedure must be repeated for the other three edges of the 8x8 blocks.

In carrying out a simulation in parallel we must be careful not to violate detailed balance. On a parallel machine we cannot test every link variable simultaneously, although such a procedure would appear to make maximum use of the parallelism. However, we can update simultaneously those variables which are not connected by the action, and it is clearly important to find the largest such subset of non-interacting variables to update at the same time. On a two-dimensional lattice gauge theory, of which a section is illustrated in Figure 13, it is quite straightforward to see that the optimum pattern is achieved by updating link variables in any one direction in a chequerboard pattern, as given by eq.(A.3) and indicated in Figure 13 by bold type. This pattern generalizes to four dimensions where we can likewise label sites as being either even or odd depending upon the sum $n_1+n_2+n_3+n_4$ of the position vectors of the site. We can then consider simultaneously updating all the links in a given direction originating from either even sites or odd sites. In this way we preserve detailed balance and it is

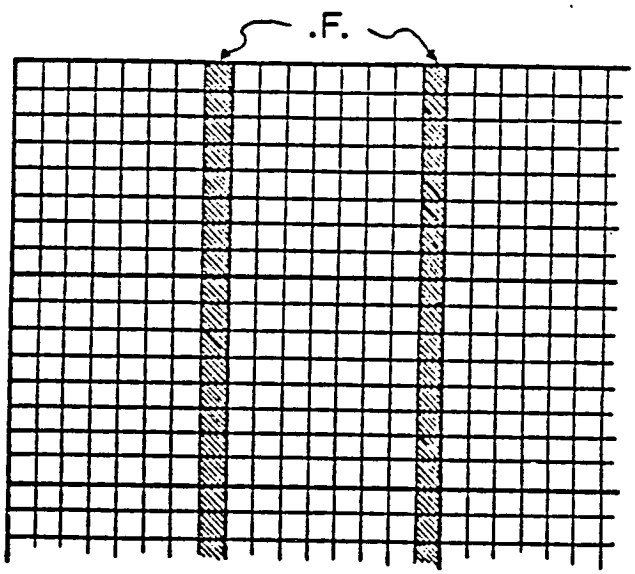



Fig. 12

Figure 12 Eastern boundary mask for 8x8 blocks, corresponding to LE=ALTC(8).LEQ.SHWC(ALTC(8),1).

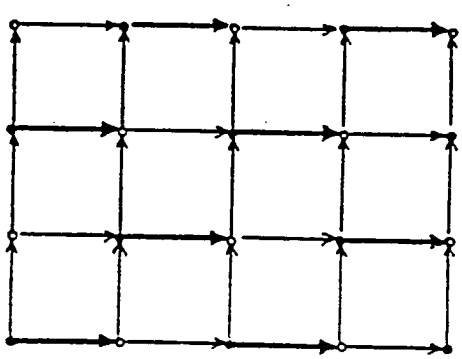


Fig. 13

Figure 13 A two-dimensional lattice: the links shown in bold-face may be updated simultaneously.

possible to update one-in-eight links simultaneously. The mask needed to define even and odd sites is a 'chequerboard of chequerboards', illustrated in Figure 14 and defined by the statement

```
LMASK=(ALTR(1).LEQ.ALTC(1)).LEQ.(ALTR(8).LEQ.ALTC(8))    (A.8)
```

Thus in a single complete sweep through the lattice in a simulation, all four directions of the gauge field and both masks in each direction need to be considered for update. In order not to lose out in efficiency when using the masks it is possible to distribute the matrix multiplies over all the PE's (i.e. some of the intermediate steps of the calculation are carried out on sites not being considered for updating).

In the two-dimensional Metropolis pseudo-fermion procedure discussed in this thesis the pseudo-fermionic action involved not nearest neighbour interactions but rather next-nearest neighbour interactions. Thus the optimum update pattern was different since any sites two spaces apart could not be updated simultaneously. In the case where the mass term was local there were no nearest neighbour interactions and consequently the update pattern consisted of pairs of neighbouring sites scattered around the lattice corresponding to the pattern

```
LMASK=(ALTR(2).LEQ.ALTC(2)).AND.ALTC(1)          (A.9)
```

thus giving an update pattern of one-in-four. When a one-link mass term is introduced the nearest neighbours in that direction clearly become connected by the action. However, the nearest neighbours in the direction orthogonal to the mass term remains uncoupled and it is thus possible to retain the update pattern given above. The same general features are true of the four dimensional case.

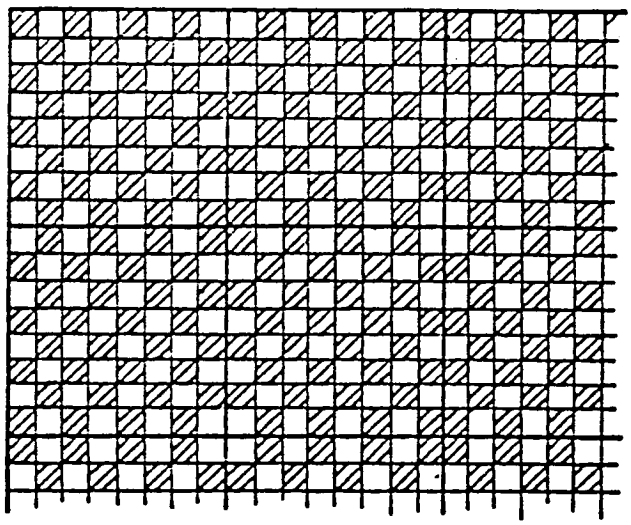


Fig.14

Figure 14 Illustration of the even/odd mask for an $8^4$ lattice:
LMASK=(ALTR(1).LEQ.ALTC(1)).LEQ.(ALTR(8).LEQ.ALTC(8)).

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