SPIN AND GAUGE FIELDS ON A LATTICE

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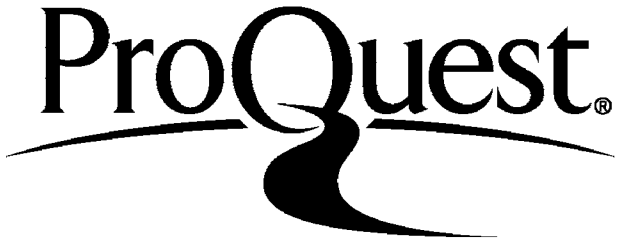

SPIN AND GAUGE FIELDS ON A LATTICE

ABSTRACT

Formulating quantum field theories on a lattice provides one way of controlling the divergences that appear in the calculation of physical quantities for these theories. At the same time the formal analogy with statistical mechanics may be exploited, in particular a continuum field theory exists only at a critical point of a statistical mechanical system.

Chapter one begins with a review of Wilson's proposal for placing gauge (local) invariant theories on a lattice, whereby quark confinement emerges as a natural consequence. The possibilities for phase transitions and spontaneous symmetry breaking in global and locally invariant theories are discussed.

Methods of calculation in lattice theories are introduced, in particular the mean field theory and Monte Carlo methods of integration.

In Chapter two those methods are applied to a globally invariant spin theory - the O(n) generalised Heisenberg model. Details of high and low temperature expansions are also given. Although much is already known about such systems we are able here to check the usefulness of our methods. In addition, the Heisenberg model is to be found at one of the limits of the system in Chapter four.

Chapter three is concerned with locally invariant pure gauge theories in four dimensions. Monte Carlo simulations are compared for the abelian U(1) theory and the non-abelian SU(3). In the U(1) case we use a finite scaling argument to suggest a second-order phase transition separating 'Maxwell' and confining regions. In SU(3) the situation is unclear, but is not inconsistent with confinement for all values of the coupling.

In Chapter four, a two coupling constant model is defined of U(1) gauge fields coupled to n-component complex matter (spin) fields. The action is then invariant to global U(n) transformations as well as local U(1). The model interpolates between pure U(1) gauge theory, a lattice version of the gauge invariant CP^{n-1} model, and the O(2n) Heisenberg model. The phase diagram is mapped out in the two coupling constant space and 'masses' are calculated in the various regions.

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Note 1

The mass calculations of Chapter four are due to Simon Duane (see attached paper 3) but have been included here for completeness.

Note 2

The computer simulations of Chapter three were initiated by K.J.M. Moriarty (see attached papers 1 and 2).

CONTENTS

Attached publications

R.C. Edgar, L. McCrossen and K.J.M. Moriarty, The Specific Heat of SU(3) Lattice Gauge Theory, J. Phys. G7, L85 (1981).

R.C. Edgar, L. McCrossen and K.J.M. Moriarty, Monte Carlo Simulation of U(1) Lattice Gauge Theory, Computer Phys. Communications 22, (1981) 433.

S. Duane, R. Gibson and L. McCrossen, CP^{n-1} Coupled to Gauge Fields: Mean Field Theory and Monte Carlo Results, Phys. Letters, 116B (1982) 44.

CHAPTER ONE INTRODUCTION

1. Gauge theories

The relativistic quantum field theories now dominating theoretical particle physics are based on the concept of local gauge invariance [1,2,3]. The principle has been most successfully applied to quantum electrodynamics (Q.E.D.), the gauge theory for Dirac particles based on the abelian group U(1). The addition of scalar fields (Higgs particles) and the idea of spontaneous symmetry breaking has since led to the successful unification of electromagnetism with the weak nuclear force [1,2].

The generalization of the idea of local gauge invariance to include arbitrary non-abelian Lie groups leads to the well known Yang-Mills theories [4]. In particular the SU(3) colour theory of quarks, known as quantum chromodynamics (Q.C.D.), is thought to govern the behaviour of the strong nuclear force [5,6,7].

There is much compelling theoretical and experimental evidence in favour of Q.C.D. [8]. One important property of non-abelian gauge theories in four dimensions is that of 'asymptotic freedom'. This idea suggests weaker interactions at smaller distances and is well supported by experiment. One might then expect stronger forces at larger distances and the possibility of quark confinement. It is this last property that occurs very naturally in the lattice gauge theories we discuss.

2. The lattice cutoff

In the Feynman path integral formulation of a general quantum field theory, perturbation expansions are made in order to predict physical quantities [2,9]. The coefficients in the expansion may

contain divergent expressions which in many cases are understood through the process of renormalization [1,2,3,9].

Ultraviolet divergences (from integrals diverging for large momentum) may firstly be 'regularized' by a modification of the integral - for instance a momentum cutoff Λ_c may be introduced, or alternatively the dimensionality may be altered. The divergent parts of these integrals may be cancelled (formally) order by order in the perturbation series by 'renormalizations' of the fields and coupling constant.

If in addition there are conditions under which the renormalized coupling constant becomes small then one might expect the leading terms in the expansion to be significant.

A theory is 'asymptotically free' if the renormalized coupling constant $g(\Lambda_c)$ tends to zero as the momentum cutoff Λ_c grows to infinity. In Q.C.D. this means that quarks are less tightly bound at short distances. In Wilson's lattice gauge theory [10,11,12,13, 14,15] one is able to probe the strong coupling regime where confinement is expected to occur.

On the lattice a natural ultraviolet cutoff is provided by the spacing a. This regularization scheme is non-perturbative in the sense that ultraviolet divergences are controlled in a manner independent of Feynman diagrams.

Consider firstly the d-dimensional infinite volume lattice Fourier transform, which should reduce to the ordinary Fourier transform as $a \to 0$:

$$\tilde{\phi}_p := c \sum_{n=-\infty}^{+\infty} e^{-ip.n} \phi_n \qquad 1.1$$

where $p = p_\mu = (p_1, \ldots, p_d)$

and the integer lattice sites are labelled*

$$n = n_\mu = (n_1, \ldots, n_d)$$

C is an arbitrary constant.

Since space is discrete the momentum space is periodic and so inversion of (1.1) is by

$$\phi_n = \frac{1}{C} \int_{-\pi}^{+\pi} \frac{d^d p}{(2\pi)^d} e^{ip.n} \tilde{\phi}_k \qquad 1.2$$

To see the cutoff, physical distances and momenta are introduced by specifying a lattice spacing a. Then we write

$$x = na$$
$$k = p/a \qquad 1.3$$

so that (1.2) becomes

$$\phi_x = C a^d \int_{-\pi/a}^{+\pi/a} \frac{d^d k}{(2\pi)^d} e^{ik.x} \tilde{\phi}_k \qquad 1.4$$

Putting $C \alpha a^{-d}$ and letting $a \to 0$ then reproduces the ordinary Fourier transform.

Equation 1.4 shows that the lattice has the effect of cutting off the momentum integral at $\Lambda_c = \pi/a$ - wavelengths of less than twice the lattice spacing have no meaning. (Note that in general the cutoff may not be the same as the usual momentum cutoff since the cutoff there is introduced after the angular integrations have

* In subsequent sections subscript x will be used rather than n to denote lattice sites.

been performed). One is interested in conditions under which the momentum cutoff is large, that is the lattice spacing appears small compared to physical length scales.

Finally, notice that in restricting the lattice to finite size N and imposing periodic boundary conditions $\phi_n = \phi_{n+N}$ on (1.2) one finds momentum is discretized:

$$p_\mu = 0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \ldots, \pm\frac{(N-2)\pi}{N}, \pm\pi \quad \text{for even } N$$

$$0, \pm\frac{2\pi}{N}, \pm\frac{4\pi}{N}, \ldots, \pm\frac{(N-3)\pi}{N}, \pm\frac{(N-1)\pi}{N} \quad \text{for odd } N. \qquad 1.5$$

3. Wilson's lattice gauge theory

As with any cutoff prescription, a renormalizable field theory may be constructed in any way that leaves the physics of the theory (when the cutoff is removed) independent of the details of the regulator. With the cutoff in place however, terms may be added to the Lagrangian which do not contribute in the continuum limit. The elegant formulation proposed by Wilson [10] is special because continuum fields with values in a Lie algebra are replaced by field variables taking their values in the corresponding Lie group. In this way, local gauge invariance is kept as an exact symmetry in the mathematically well-defined system.

In Chapter three pure U(1) and SU(3) lattice gauge theories in four dimensions are compared. The lattice U(1) action is easily shown to reduce to the conventional Q.E.D. action as the lattice spacing is taken to zero. In Chapter four the U(1) gauge field is coupled to n-component scalar fields to give a lattice version of scalar Q.E.D.

In order to review the properties of Wilson's lattice gauge theory we now consider pure SU(3). Consider the Q.C.D. Lagrangian in four-dimensional Euclidean space [1], restricting attention to pure Yang-Mills fields.

$$\mathcal{L} = -\frac{1}{4} \sum_{a=1}^{8} \sum_{\mu,\nu=1}^{4} F^a_{\mu\nu}(x)\, F^a_{\mu\nu}(x) \qquad 1.6$$

with

$$F^a_{\mu\nu}(x) = \partial_\mu A^a_\nu(x) - \partial_\nu A^a_\mu(x) - g \sum_{b,c} f^{abc} A^b_\mu(x) A^c_\nu(x)$$

The f^{abc} are the structure constants of SU(3) [16] satisfying

$$[\lambda^a, \lambda^b] = 2i \sum_{c=1}^{8} f^{abc} \lambda^c \qquad 1.7$$

where λ^a are the eight generators of SU(3), conventionally chosen to be the Gell-Mann matrices. The dimensionless parameter g plays the role of a coupling constant. The gauge fields $A^a_\mu(x)$ are vector fields carrying an index of the adjoint representation of the group SU(3).

Letting $A_\mu(x)$ denote the corresponding element of the Lie algebra

$$A_\mu(x) = \sum_{a=1}^{8} \frac{\lambda^a}{2} A^a_\mu(x) \qquad 1.8$$

the Lagrangian (1.6) is then invariant under the following transformations :

$$A_\mu(x) \to {}^{g}A_\mu(x) = g(x)\, A_\mu(x)\, g^{-1}(x) + \frac{i}{g} [\partial_\mu g(x)] g^{-1}(x) \qquad 1.9$$

where $g(x)$ denotes an element of SU(3). The full Lagrangian would contain in addition to (1.6), scalar or fermion fields coupled to the gauge field in a manner invariant to (1.9).

In Wilson's lattice formulation the gauge fields are thought of as residing on the links of a hypercubical lattice with spacing a. The links are specified by a lattice site and a forward direction μ along a link out of the site. The pure gauge theory action reads: (See for example ref. [13] for proposals concerning the inclusion of fermion fields)

$$S(g,a) = \frac{1}{2g^2} \sum_{x} \sum_{\substack{\mu,\nu=1 \\ \mu\neq\nu}}^{4} \mathrm{Tr}[U_x^{\mu} U_{x+\hat{\mu}}^{\nu} U_{x+\hat{\nu}}^{\mu\,-1} U_x^{\nu\,-1} + \mathrm{h.c.}] \qquad 1.10$$

where $\hat{\mu}$ steps one lattice spacing in the μ direction. (The $\hat{}$ notation is dropped from now on). The U_x^{μ}'s are SU(3) matrices, which may be written in the representation

$$U_x^{\mu} = \exp[\, i a g A_x^{\mu} \,] \qquad 1.11$$

where $$A_x^{\mu} = \sum_{a=1}^{8} \frac{\lambda^a}{2} A_x^{a\,\mu}$$

(Note that A_x^{μ} is bounded since SU(3) is compact).

The four U's in equation 1.10 then form an elementary square or 'plaquette' and the sum is over all such plaquettes on the lattice. Imagining a set of local transformations on the site forming the plaquettes, the action (1.10) is invariant under

$$U_x^{\mu} \to {}^{g}U_x^{\mu} = g_x\, U_x^{\mu}\, g_{x+\mu}^{-1} \qquad 1.12$$

To see the corresponding continuum theory the lattice 'difference operator' is defined:

$$\Delta_\nu A^\mu_x := A^\mu_{x+\nu} - A^\mu_x \qquad 1.13$$

For small a Δ_μ/a approximates a derivative ∂_μ. If the fields are smooth (but see later in this section) a Taylor expansion may be made:

$$A^\mu_{x+\nu} = A^\nu_x + \Delta_\mu A^\nu_x$$

$$= A^\nu_x + a\partial_\mu A^\nu_x + O(a^2) + \ldots \qquad 1.14$$

Using (1.11) the four U^μ_x's in the action may be rewritten as a product of exponentials. Repeated use of the Baker-Campbell-Hausdorff formula

$$e^{AB} = e^{A+B + \frac{1}{2}[A,B] + \ldots} \qquad 1.15$$

and equation 1.14 brings the expression for the U's into the form of a single exponential

$$\exp\{i a^2 g(\partial_\mu A^\nu_x - \partial_\nu A^\mu_x + i g [A^\mu_x , A^\nu_x]) + O(a^3)\ldots\}$$

$$= \exp\{ i a^2 g \sum_d (\partial_\mu A^{\nu d}_x - \partial_\nu A^{\mu d}_x - g f^{abc} A^{\mu b}_x A^{\nu c}_x) \frac{\lambda^d}{2} + O(a^3) \ldots\} \qquad 1.16$$

Then (1.10) becomes

$$S(g,a) = \frac{1}{2g^2} \sum_{\times} \sum_{\mu,\nu} \mathrm{Tr} \exp\{i a^2 g \sum_a F^{\mu\nu a}_x \frac{\lambda^a}{2} + O(a^3)\ldots\} \qquad 1.17$$

Expanding the exponential in (1.17) the Tr 1 term has no dynamics and may be dropped. The term linear in $F^{\mu\nu a}_x$ is traceless and so we have

$$S(g,a) = \frac{1}{2g^2} \sum_{x} \sum_{\mu,\nu} \{ - a^4 g^2 [\sum_{a} \sum_{b} Tr(\frac{\lambda^a}{2} \frac{\lambda^b}{2}) F_x^{\mu\nu a} F_x^{\mu\nu b}] + O(a^5) \ldots \} \qquad 1.18$$

Finally, replacing

$$\sum_{x} \rightarrow a^{-4} \int d^4x \qquad 1.19$$

in the limit $a \rightarrow 0$ reproduces the continuum action (1.6)

$$\lim_{a \rightarrow 0} S(g,a) = \int d^4x \, (-\frac{1}{4} \sum_{a} \sum_{\mu,\nu} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x)) \qquad 1.20$$

By a similar argument the transformation (1.12) becomes the continuum transformation equation 1.9.

Note that if $d \neq 4$ a rescaling of the dimensionless coupling constant or fields by a power of a is required to keep the action dimensionless. The existence of dimensionless parameters in the action indicates the renormalizability of the model in four dimensions [1] (also see Chapter two).

Notice that equation 1.14 is only valid for smoothly varying classical fields [11] - fluctuations in the full quantum theory will only become unimportant when the action is large and negative. Hence in the quantum formulation that we now review, the 'naive' limit $a \rightarrow 0$ may not approach the correct continuum theory for all values of the coupling.

In the lattice quantum theory the generating functional Z looks like the partition function for a statistical mechanical system (see next section).

$$Z = \int \prod_{\text{links}} D U \exp\{S(g,a)\} \qquad 1.21$$

where $D U$ is the group invariant measure [16]. Gauge invariant expectation values $< Q >$ are given by

$$< Q > = Z^{-1} \int \prod_{\text{links}} Q \exp\{S(g,a)\} \qquad 1.22$$

One important quantity is the 'Wilson loop' [1]:

$$Q_W = \mathrm{Tr} \Big(\prod_{\substack{T \times R \\ \text{planar loops}}} U \Big) \qquad 1.23$$

A strong coupling expansion (see Chapter three) gives

$$< Q_W > \; \alpha \; (\frac{1}{g^2})^{TR} + \text{higher orders} \qquad 1.24$$

For $T >> R$ the closed current loop $< Q_W >$ may be interpreted as the ratio of the partition function with external charges to the partition function without them. The system is seen as containing a static charge at $x = R$ separated from its antiparticle at $x = 0$. We write

$$< Q_W > = \frac{Z[J]}{Z[0]} \sim \exp\{(E[J] - E[0])\, T\} \qquad 1.25$$

A study of the transfer matrix [12] shows that $E[J]$ represents the lowest lying energy level for the system. Since the charges are static the energy difference in (1.25) is pure potential. Using (1.24) one finds the confining potential

$$V(R) \;\; \alpha \;\; R \qquad 1.26$$

If this picture could be extended to include quarks [17] we see that confinement would emerge very naturally in the lattice theory at strong coupling.

4 Statistical mechanics and phase transitions.

Much of our understanding of lattice gauge theories is derived from a knowledge of critical phenomena in spin systems [18]. These spin theories correspond to globally invariant spin (matter) theories in the continuum. An important example of a spin theory is the O(n) generalised Heisenberg model discussed in Chapter two. Like four-dimensional non-abelian gauge theories this model is asymptotically free in two dimensions for $n > 2$.

Familiar objects in field theory are associated with statistical mechanical quantities [11, 19], for instance the two-point function is identified on the lattice as the spin-spin correlation function C(r) (see next section). From this a further relation may be derived:

$$\xi a = \frac{1}{M_R} \qquad 1.27$$

where M_R is the renormalized mass of the field theory. ξ is the correlation length of the statistical system, and in some sense characterizes correlations between spins separated by distance r.

For a general theory a phase diagram might be drawn showing the dependence of some quantity $\langle Q \rangle$ on the bare coupling g. Equation 1.27 tells us that a sensible continuum theory will be found only at places where $\xi \to \infty$. By holding M_R fixed and allowing the spacing a to go to zero an effective coupling g(a) is defined (and hence a whole sequence of lattice theories). If a continuum limit exists, then as the lattice cutoff is removed g(a) should tend in some way towards a point where the scale of correlation becomes unbounded.

In the language of statistical mechanics, such points are examples

of critical behaviour of the system. (See Chapter two). If at some temperature T_c ($T \alpha g$) ξ tends to infinity accompanied by a spontaneous magnetization (spontaneous symmetry breaking) then the system is said to have undergone a second-order phase transition. This situation occurs for example in $O(n)$ if n and d are large. Alternatively, the scale of correlations may diverge without the occurrence of a spontaneous magnetization, as for example in the $O(2)$ system in two dimensions.

There is unfortunately, no more hope of solving exactly the lattice theory than a conventional field theory. In addition, in the region of large ξ, correlation functions become difficult to study - finite order small and large coupling expansions may leave their domain of validity. However, the lattice system is amenable to a powerful non-perturbative approximation - Monte Carlo simulation (see section six). Wilson [20] and Creutz [21] have used this technique in conjunction with renormalization group ideas [9,11,19,22] to study non-abelian lattice gauge theories. For an example of Wilson's approach applied to a spin theory, see ref. [23].

In a gauge theory a physical observable such as the string tension $\chi(g)$ may be extracted from combinations of Wilson loops. By increasing the size of the loops and holding χ fixed in the process, the lattice spacing is effectively reduced. In this way Creutz attempts to match the strong coupling behaviour (equation 1.26) of the string tension in lattice Q.C.D. to the known asymptotic freedom prediction at weak coupling.

In Chapter three we compare Monte Carlo simulations of $U(1)$ and $SU(3)$ four-dimensional lattice gauge theories. If the (full) $U(1)$

lattice theory as $a \to 0$ is to describe conventional Q.E.D. then the confining properties at strong coupling should not persist for all values of the coupling. Thus a transition is expected to occur at some finite g_c. Below g_c the continuum limit of the lattice theory should contain free electrons. On the other hand, if Creutz's approach is not misleading, the strong coupling behaviour in SU(3) should continue smoothly into the region of vanishing coupling, as has been found in the O(3) spin model in two dimensions [23].

In Chapter four matter fields are coupled to the U(1) gauge fields and we discuss the possibility of a 'Higgs' phase in addition to confining and 'Maxwell' phases.

5 Mean field theory

A very useful guide to the lattice physics is provided by the mean field approximation. Some details of this method are given in Chapter two. In this section we show briefly how masses might be calculated in this approximation and how Goldstone's theorem applies.

Consider the O(n) Heisenberg model of Chapter two, consisting of n-component spins $\phi_x = (\phi_x^1, \phi_x^2, \ldots \phi_x^n)$ of unit length situated at the sites of the lattice.

The action with sources J_x reads

$$H = \sum_{x,\mu} \phi_{x+\mu} \phi_x + \sum_x \phi_x \cdot J_x \,. \qquad 1.28$$

The partition function is

$$Z(\beta) = \int \prod_x D\phi_x \exp\{\beta H\} \qquad 1.29$$

where $\beta = 1/T$ and a suitable measure $D\phi_x$ has been defined. Expectation values $<Q>$ are given by

$$<Q> = Z^{-1} \int \prod_x D\phi_x \; Q \exp\{\beta H\} \qquad 1.30$$

The key to the mean field idea lies in defining a mean field h_x consistent with (1.30). When $Q = \phi_x$, h_x is thought of as the average field over nearest neighbours $y(x)$. For the Heisenberg model (see Chapter two)

$$h_x = \beta \sum_{y(x)} <\phi_y> + J_x \qquad 1.31$$

$$= 2d\,\beta <\phi_x> + J_x \; . \qquad 1.32$$

The partition function becomes

$$Z(\beta) = \int D\phi \; \exp\{\phi \cdot h_x\} \qquad 1.33$$

with the average field

$$<\phi_x> = \int D\phi \; \phi_x \; \exp\{\phi \cdot h_x\} \qquad 1.34$$

In order to extract masses, consider the connected spin-spin correlation function

$$<\phi_x^i \cdot \phi_y^j>_c := <\phi_x^i \cdot \phi_x^j> - <\phi_x^i><\phi_x^j> \qquad 1.35$$

Then we write

$$<\phi_x^i \cdot \phi_x^j>_c = \frac{\partial <\phi_x^i>}{\partial J_x^j}$$

$$= \frac{d\langle\phi_x^i\rangle}{d\, h_x^k} \quad \frac{\partial\, h_x^k}{\partial\, J_y^j} \tag{1.36}$$

Using (1.34) equation 1.36 becomes

$$\langle \phi_x^i \cdot \phi_y^j \rangle_c = [\langle \phi_x^i \cdot \phi_x^k \rangle - \langle \phi_x^i \rangle \langle \phi_x^k \rangle] \frac{\partial\, h_x^k}{\partial\, J_y^j}$$

$$= \langle \phi_x^i \cdot \phi_x^j \rangle_c [\beta (\Delta_x^2 + 2d) \frac{\partial \langle \phi_x^k \rangle}{\partial\, J_y^j} + \delta_{kj}\, \delta_{xy}] \tag{1.37}$$

Δ^2 is the lattice Laplacian defined by

$$\Delta_x^2 f(x) := \sum_{y(x)} f(y) - 2d\, f(x) \ .$$

The last equation is derived by noting that equation 1.31 may be written

$$h_x = \beta (\Delta_x^2 + 2d) \langle \phi_x \rangle + J_x \tag{1.38}$$

Finally, the correlation function is expressed as

$$\langle \phi_x^i \cdot \phi_y^j \rangle_c = \langle \phi_x^i \cdot \phi_x^k \rangle_c [\beta(\Delta_x^2 + 2d) \langle \phi_x^k \cdot \phi_x^j \rangle_c + \delta_{kj}\, \delta_{xy}] \tag{1.39}$$

or

$$[-\Delta_x^2\, \delta_{ij} + (M^2)_{ij}] \langle \phi_x^j \cdot \phi_y^k \rangle_c = \beta^{-1}\, \delta_{ik}\, \delta_{xy} \tag{1.40}$$

Equation 1.40 looks like a free particle wave equation with mass matrix M^2 :

$$M^2 = (\beta \langle \phi_x^i \cdot \phi_x^j \rangle_c)^{-1} - 2d\, \delta_{ij} \tag{1.41}$$

where the quantity $< \phi_x^i \cdot \phi_x^j >_c$ is easily evaluated in the mean field approximation.

In the case of spontaneous symmetry breaking (see Chapter two) Goldstone's theorem applies. Here at most one component σ_x of $\phi_x = (\sigma_x, \pi_x^2, \pi_x^2, \ldots, \pi_x^{n-1})$ gains a non-zero expectation value. Equation 1.41 gives one massive scalar

$$\mu_\sigma^2 = (\beta < \sigma_x \cdot \sigma_x >_c)^{-1} - 2d \qquad 1.42$$

In addition there are $n-1$ massless Goldstone bosons:

Selecting one component π of $\underline{\pi}^1$ we have (with J_x set to zero) from (1.33)

$$< \pi_x^2 > = Z^{-1} \int D\phi \; \pi_x^1 \exp\{2d\beta < \sigma_x > \cdot \sigma\} \qquad 1.43$$

Consider equation 1.29 invariant to global rotations

$$\phi_x \rightarrow \phi_x' = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \phi_x \qquad 1.44$$

The infinitesimal form of (1.44) is

$$\phi_x' = [1 + \varepsilon \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}] \phi_x \qquad 1.45$$

Thus we may write

$$\begin{aligned} \delta_\sigma &= -\varepsilon \pi^1 \\ \delta\pi &= \varepsilon \sigma \end{aligned} \qquad 1.46$$

and the Ward identity [9] may be derived

$$0 = \varepsilon[< \sigma_x > - 2d\beta < \pi_x^1 \cdot \pi_x^1 > < \sigma_x > + 2d\beta < \pi_x^1 > < \pi_x^1 > < \sigma_x >] \qquad 1.47$$

$$= \varepsilon [< \sigma_x > - 2d\beta < \pi^1_x \cdot \pi^1_x >_c < \sigma_x >]$$

$$= \varepsilon < \sigma_x > \mu^2_\pi \beta < \pi^1_x \cdot \pi^1_x >_c \qquad 1.48$$

Now $\beta < \pi^1_x \cdot \pi^1_x > > 0$ always, hence if $< \sigma_x > \neq 0$ we have the Goldstone boson

$$\mu^2_\pi = 0 \qquad 1.49$$

6 Monte Carlo methods.

The aim of a Monte Carlo simulation [24] is to obtain an approximation to the expectation value

$$< Q > = Z^{-1} \int D\phi \, Q(\phi) \exp\{ S(\phi) \} \qquad 1.50$$

where the ϕ's form a set of numbers (either spins on the sites of the lattice or gauge variables on the links). On a finite lattice the set is finite and a full description of a configuration may be written down. In the case of continuous groups however, there are still an infinite number of configurations. In a Monte Carlo simulation the full integral is approximated by a sum over a finite sequence of states. In order to obtain a good approximation to (1.50) the density of states in the sequence should approach

$$\rho(\phi) = \exp\{ S(\phi) \} / Z \qquad 1.51$$

i.e. the probability density of encountering any configuration is proportional to the Boltzmann weighting $\exp\{S(\phi)\}$.

Successive configurations are generated from proceding ones using a specific algorithm. (Usually one seeks the aid of a computer for storing and updating variables - for example, there are 1024 links on

a 4^4 lattice). The probability of obtaining a configuration ϕ' from ϕ may be specified as $P(\phi', \phi)$.

The choice of $P(\phi', \phi)$ is not unique [25]. Many algorithms change one variable (site or link) at a time satisfying a condition of 'detailed balance':

$$P(\phi', \phi)\, e^{-\beta S(\phi)} = P(\phi, \phi')\, e^{-\beta S(\phi')} \qquad 1.52$$

It may be shown [26] that any algorithm satisfying equation 1.52 will bring an ensemble of configurations into the correct equilibrium state defined by equation 1.51. To understand this we consider a particular algorithm.

In Chapters two and four we use the algorithm of Metropolis [27], well known in statistical mechanics. A random generator (designed to optimize convergence - see Chapter two) is used to suggest a new configuration $\phi'_B = B(\phi)$. ϕ'_B then replaces ϕ if

$$\rho(\phi'_B) > x\, \rho(\phi) \qquad 1.53$$

where x is a number uniformly distributed between zero and one. Otherwise ϕ is kept and ϕ'_B is discarded.

The probability that $B(\phi)$ suggests ϕ' is written $B(\phi', \phi)$ so that

$$P(\phi', \phi) = \begin{cases} B(\phi', \phi) & \text{if } \rho(\phi') \geq \rho(\phi) \\ B(\phi', \phi)\, \dfrac{\rho(\phi')}{\rho(\phi)} & \text{if } \rho(\phi') < \rho(\phi) \\ \text{The remainder } (B_R \text{ say}) & \text{if } \phi' = \phi \text{ (important for discrete groups)} \end{cases} \qquad 1.54$$

Note that if the following condition holds true for the particular algorithm (see Chapter two):

$$B(\phi',\phi) = B(\phi, \phi') \qquad 1.55$$

then using equation 1.54 we see that the detailed balance equation 1.52 is satisfied.

Now assuming (1.55) and using (1.54) we have

$$\sum_{\phi'} P(\phi,\phi')\rho(\phi') = \sum_{\{\phi':\rho(\phi')\geq\rho(\phi)\}} B(\phi,\phi')\rho(\phi') + \sum_{\{\phi':\rho(\phi')\geq\rho(\phi)\}} B(\phi,\phi')\rho(\phi)$$

$$+ B_R\,\rho(\phi)$$

$$= \sum_{\phi'} P(\phi',\phi)\rho(\phi) = \rho(\phi) \qquad 1.56$$

Denoting the m-step probability as $P_m(\phi',\phi)$ we have

$$\sum_{\phi''} P(\phi',\phi'')\,P_m(\phi'',\phi) = P_{m+1}(\phi',\phi) \qquad 1.57$$

Hence as $m \to \infty$ the desired result is obtained:

$$P_m(\phi',\phi) \to \rho(\phi') \qquad 1.58$$

Note that the detailed balance condition is sufficient but not necessary to achieve the correct target distribution $\rho(\phi')$. In Chapter three we use the more intuitive 'heat bath' method of Creutz (see Chapter three and Appendix B). Here the new spins or links are selected randomly from the group space with a weighting given by the Boltzmann factor

$$P(\phi') \sim e^{-\beta S(\phi')} \qquad 1.59$$

In this way equation 1.51 is satisfied, yet for this algorithm

detailed balance holds only if the spins to be updated are selected from random positions on the lattice [28].

Since essentially an experiment is being conducted one considers the expectation value $\langle \bar{Q} \rangle$ of the average of $Q(\phi)$ over a sequence of configurations $\phi_o, \ldots, \phi_N$. We conclude by showing that if equation 1.58 holds then $\langle \bar{Q} \rangle$ approaches $\langle Q \rangle$ as $N \to \infty$.

The expectation value of the sequence average is

$$\langle \bar{Q} \rangle = \sum_{\substack{\{\text{all possible} \\ \text{sequences} \\ \phi_o, \ldots, \phi_N\}}} P(\phi_N, \phi_{N-1}) \ldots P(\phi_1, \phi_o) \frac{1}{N} \sum_{n=1}^{N} Q(\phi_n) \qquad 1.60$$

$$= \frac{1}{N} \Big[\sum_{\phi_1} Q(\phi_1) P(\phi_1, \phi_o) + \sum_{\phi_1, \phi_2} Q(\phi_2) P(\phi_1, \phi_o) P(\phi_2, \phi_1) + \ldots \Big]$$

$$= \frac{1}{N} \Big[\sum_{\phi} Q(\phi) P(\phi, \phi_o) + \sum_{\phi} Q(\phi) P_1(\phi, \phi_o) + \ldots \Big]$$

$$= \frac{1}{N} \sum_{\phi} \sum_{n=1}^{N} Q(\phi) P_n(\phi, \phi_o)$$

$$= \sum_{\phi} Q(\phi) \Big[\rho(\phi) + \frac{1}{N} \sum_{n=1}^{N} D_n(\phi, \phi_o) \Big] \qquad 1.61$$

where D_n measures the 'distance' of P_n from the equilibrium distribution.

Let λ be a positive constant such that

$$| D_n | \leq e^{-\lambda n} \qquad 1.62$$

so

$$\left| \sum_{n=1}^{\infty} D_n \right| < \frac{1}{\lambda} \qquad 1.63$$

and hence $\langle \bar{Q} \rangle$ approaches $\langle Q \rangle$ as N tends to infinity.

Finally, since $\langle \bar{Q} \rangle$ is a sum over distributions, the Central Limit Theorem applies for large N. Standard error estimates ($\sim 1/\sqrt{N}$) may then be made on $\langle \bar{Q} \rangle$ [24].

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A SURVEY OF METHODS - THE O(n) HEISENBERG MODEL

CHAPTER TWO

We begin with the generalised Heisenberg model [1-4] for two reasons. Firstly, the model is of great interest in statistical mechanics. Much is already known about such systems, so it is easier to check the usefulness of our methods. Secondly, the spin-gauge model of Chapter four is, at one of its limits, gauge equivalent to the Heisenberg model.

The corresponding continuum field theory is the O(n) non-linear σ-model*. This model is non-renormalizable according to usual criteria in four-dimensional space-time. On the other hand, the two-dimensional case is renormalizable [5] and enjoys a number of features in common with four-dimensional non-abelian gauge theories [5,6,7].

1. Definition

We consider a square periodic lattice in d dimensions with N^d sites and spacing a. To each site we associate an n-component spin vector $\phi_x = (\phi_x^1, \phi_x^2, \ldots, \phi_x^n)$. Each site is coupled only to its nearest neighbours in all directions μ, with strength J. Thus the Hamiltonian

$$H = J \sum_{x,\mu} \phi_{x+\mu} \cdot \phi_x \qquad 2.1$$

is invariant to global rotations of the spins.

Properties of the statistical mechanical system are extracted from the partition function

$$Z(\beta) = \int \prod_x D\phi_x \, \delta(\phi_x^2 - 1) \exp\{-\beta H\} \qquad 2.2$$

*See Chapter four for reference to general non-linear σ-models.

and various expectation values

$$< Q > = Z^{-1} \int \prod_x D\phi_x \, \delta(\phi_x^2 - 1) \, Q \exp\{-\beta H\} \qquad 2.3$$

where $\beta = J/_T$, T = temperature .

The fixed length condition $\phi_x^2 \equiv 1$ is incorporated into the measure here and leads to non-trivial interactions.

2. High and low temperatures.

Systematic expansions of equation (2.3) may be made for high and low T. These methods are reviewed in appendix A as they will be useful in Chapter four.

The following results are for the average energy density E and may be compared with the Monte Carlo data in Fig. 1a:

$$E(\beta) = < \frac{1}{N_\ell} \sum_{x,\mu} \phi_{x+\mu} \, \phi_x > = < \phi_{x+\mu} \, \phi_x > \qquad 2.4$$

since the lattice is translation invariant. (N_ℓ is the number of links on the lattice.)

(i) High temperature (low β)

$$E(\beta) \sim \beta/n + \left[\frac{2d}{n^2} - \frac{3n+4}{n^2(n+2)} \right] \beta^3 + O(\beta^5) \ldots \qquad 2.5$$

(ii) Low temperature (high β)

$$E(\beta) \sim 1 - \frac{n-1}{2d\beta} - \frac{n-1}{8d^2\beta^2} + O(\beta^{-3}) \ldots \qquad 2.6$$

(neglecting terms $O(\beta^{-2} N_\ell^{-1})$.

The high temperature result is insensitive to the lattice size at this low order, while at low temperatures long wave-length fluctuations

are important and the calculation shows an N_ℓ dependence at order β^{-2}.

3. Phase transitions.

In the cases $d = 4$, $n = 4,6$ that we consider the space and spin dimensions are high enough that a second-order phase transition occurs at some finite T_c.

At high T the model is considered to be in the symmetric phase and $\langle \phi_x^i \rangle \equiv 0$ for all $i = 1,\ldots,n$. Define the connected spin-spin correlation function for two spins separated by distance r:

$$\begin{aligned} C(r) &= \langle \phi_{x+r} \cdot \phi_x \rangle - \langle \phi_{x+r} \rangle \langle \phi_x \rangle \\ &= \langle \phi_{x+r} \cdot \phi_x \rangle - \langle \phi_x \rangle^2 \quad \text{by translation invariance} \\ &= \langle \phi_{x+r} \cdot \phi_x \rangle \quad \text{in the symmetric phase.} \end{aligned} \tag{2.7}$$

At high T the large r behaviour is thought to be [8]

$$C(r) \sim \exp\{-r/\xi(T)\} \tag{2.8}$$

up to a power of r*.

$\xi(T)$ is known as the correlation length.

For low T a spontaneous magnetization occurs. The symmetry is broken and $\langle \phi_x^i \rangle \neq 0$ for some i. As the system is simply magnetized there are no long-range correlations and we expect

$$C(r) = \langle \phi_{x+r} \phi_x \rangle - \langle \phi_x \rangle^2 \simeq 0 \tag{2.9}$$

We shall be interested in the behaviour of systems that are close to the critical temperature Tc. In this region distant spins are highly correlated in some sense characterized by the correlation length. The critical behaviour of various other thermodynamic quantities can be represented as a set of critical indices [9].

* See section 7.

One such quantity, which will be of use in measuring distant correlations, is the magnetic susceptibility $\chi(T)$:

Add an external field J_x to H of (2.1):

$$H \to H + \sum_x J_x \cdot \phi_x = \beta \sum_{x,\mu} \phi_{x+\mu} \cdot \phi_x + \sum_x J_x \cdot \phi_x \qquad 2.10$$

Then define

$$\chi(\beta) = \frac{\delta}{\delta J_y} < \phi_x > \Big|_{J_x \equiv 0} \qquad 2.11$$

By a version of the fluctuation - dissipation theorem [2] it is easy to obtain the useful result

$$\chi(\beta) = < \sum_{y \neq x} \phi_y \cdot \phi_x > - < \phi_x >^2 \qquad 2.12$$

Clearly the sum in (2.12) will show up the long range contribution near Tc.

4. Critical region and continuum field theory

Defining the lattice 'difference operator' $\Delta_\mu \phi_x = \phi_{x+\mu} - \phi_x$, equation (2.1) looks like a lattice approximation to the Euclidean action for the contunuum $O(n)$ non-linear σ-model in field theory :

$$H = \sum_{x,\mu} [1 - \frac{1}{2}(\Delta_\mu \phi_x)^2] \, . \qquad 2.13$$

Identifying β with the inverse coupling constant $\frac{1}{g^2}$ and adding external sources, $Z(\beta)$ becomes the familiar generating functional for the Green's functions of the field theory.

For a general scalar theory, comparison of the long range behavior of $C(r)$ with the field-theoretic propagator yields the familiar relation [1,11].

$$M_R = \frac{1}{\xi a} \qquad 2.14$$

where M_R is the renormalized mass of the field theory. Equation (2.14) tells us that as $a \to 0$ finite masses will only be obtained from the lattice if the system is nearly critical.

The special status of $d = 2$ for these models is observed by making the approximation to the continuum theory for small a:

$$\begin{aligned} \partial\mu\ \phi(x) &\underset{\sim}{} \Delta\mu\ \phi_x/a \\ \int d^d x &\underset{\sim}{} a^d \sum_{x,\mu} \end{aligned} \qquad 2.15$$

Substitution into (2.13) brings out the first order power $a^{(2-d)}$. In $d = 2$ we see that H remains dimensionless without rescaling of the parameters $\phi(x)$ or g to cancel this power. This fact leads to the renormalizability of the model and the $d = 2 + \varepsilon$ expansions [4,12].

5 Approximate models.

In the vicinity of Tc the expansions of section two are of limited use and we look to ways of simplifying H itself.

One method is to take the 'Stanley limit' $n \to \infty$ (Spherical model) and make corrections in $\frac{1}{n}$ [4,13]. We might expect good results for the cases $n = 4,6$ to be considered.

An alternative is to play with the space dimensionality of the system. For example, the case $d = 1$ is informative [2] - the spins decouple in the expresion for $Z(\beta)$ so that each link (bond) gives a factor

$$\gamma\left(\frac{n}{2}\right)\ \beta^{1-n/2}\ I_{n/2-1}(\beta) \qquad \text{where } I_n \text{ is the modified}$$

Bessel function, $\gamma(q)$ is the gamma function .

There is obviously no transition here at any finite T, but a zero mass may be extracted as $T \to 0$ when the system approaches ordering and

the correlation function behaves as

$$C(r, \beta) \sim \exp\{^{-r(n-1)}/_{2\beta}\} \qquad 2.16$$

The cases $d = 2, 3, 4$ are the most physically relevant and the most difficult to study. Close to $d = 2, 4$, useful expansion have been made in $\varepsilon = d - 2$ [4,12] and in $\varepsilon = 4 - d$ [3,11].

For $d > 4$ we may rely on the other extreme $d \to \infty$-an interpretation of mean field theory where the number of nearest neighbour interactions becomes large and so behaves as some average field [2]. We shall construct a mean field theory argument as a guide to the case $d = 4$.

6. Mean field theory

The idea of a mean field theory has many interpretations [2]. From the field theoretic point of view [3] a formal perturbation expansion is made around a saddle-point approximation to $W = \ell n\, Z$. The first term W_o in this series is the mean field theory. Corrections to this lowest order indicate that the mean field approximation is certainly invalid below four dimensions while above $d = 4$ critical exponents are not modified

As a first step before making any calculations the assumption of a mean field is made self-consistent. Write the action equation (2.10) in terms of pairs of sites (x,y):

$$S = \beta \sum_{(x,y)} \phi_x \cdot \phi_y + \sum_x J_x \cdot \phi_x \qquad 2.17$$

A given ϕ_x interacts with $\sum_{y(x)} \phi_y + J_x$ where $y(x)$ denotes the 2d neighbours of the site x. The mean field h_x may then be written as some average over those neighbours :

$$h_x := \beta \sum_{y(x)} \langle \phi_y \rangle + J_x \qquad 2.18$$

Self-consistency then requires

$$\langle \phi_x \rangle = Z^{-1} \int \prod_x D\phi_x \delta(\phi_x^2 - 1)\, \phi_x \exp\{-\phi_x . h_x\}$$

$$Z(h) = \int \prod_x D\phi_x\, \delta(\phi_x^2 - 1)\, \exp\{-\phi_x . h_x\} \qquad 2.19$$

where Z is seen to decouple in a similar fashion to the case $d = 1$, and calculations are made using the single site measure

$$D\phi := D\phi_x\, \delta(\phi_x^2 - 1) \qquad \text{for all } x .$$

Symmetry breaking

Assume constant sources chosen in the 1^{st} direction and write

$$J_x = (J_x, 0, \ldots, 0)$$

$$\phi_x = (\sigma, \pi_1, \ldots \pi_{n-1})$$

so that $\langle \underline{\pi} \rangle = 0$ while $\langle \sigma \rangle \neq 0$.

Then self-consistency requires

$$\langle \sigma \rangle = Z^{-1} \int D\phi\, \sigma \exp\{-h\sigma\} \qquad 2.20$$

where $$Z(h) = \int D\phi \exp\{-h\sigma\}$$

and $$h = 2d\beta \langle \sigma \rangle + J .$$

A unique solution to eqn. (2.20) may be obtained by the following construction of the thermodynamic potential $\Gamma(\langle\sigma\rangle)$, (the Legendre transform of ω) given by the equation [3]

$$\frac{d\Gamma}{d\langle\sigma\rangle} = J \qquad 2.21$$

$$J = h - 2d\beta\langle\sigma\rangle$$

Noticing $\frac{\partial}{\partial h} \ln Z(h) = \langle\sigma\rangle$ leads to the solution (up to an irrelevant additive constant)

$$\Gamma(<\sigma>) = J <\sigma> + d\beta<\sigma>^2 - \ln Z(2d\beta<\sigma> + J) \qquad 2.22$$

with $Z(h) = \gamma(\frac{n}{2})(h)^{1-n/2} I_{n/2-1}(h)$. ($\gamma(\frac{n}{2})$ is the gamma function.

We can then minimize Γ w.r.t. $<\sigma>$ (in the absence of an external field J) by considering eqn.(2.22)and expansions of lnZ for small and large h^* .

For small β (high temperature) the minimum occurs at $<\sigma> = 0$ and the model is in its symmetric phase. At $\beta = \beta c$ two minima appear either side of $<\sigma> = 0$, but as close as we like to $<\sigma> = 0$. It is easy to show that $\beta_c = n/d$ [14].

As β is increased past the transition point the two minima move smoothly away from $<\sigma> = 0$. Thus the model has undergone a second-order (continuous) transition and is in its ordered phase.

Calculation of masses

Identifying the long range behaviour of the correlation function with the small momentum behaviour of the two-point function we may extract masses from the lattice approximation [14].

The following mean field result is derived in momentum space. In position space the result is straightforward for the Heisenberg model† but presents problems when applied to the mixed model of Chapter four.

Take the mean field h_x^i, $i = 1,2,\ldots,n$ in the absence of an external field (source):

$$h_x^i = \beta \sum_{y(x)} <\phi_y^i> \qquad 2.23$$

and consider the response of h_x^i to a small position dependent source J_x^i :

* Bessel Functions for Engineers - N.W. McLachlan - O.U.P.

† See Chapter one.

$$\delta h_x^i = \beta \sum_{y(x)} \delta \langle \phi_y^i \rangle + J_x^i \quad . \tag{2.24}$$

Working in momentum space (see appendix A) :

$$J_x^i \rightarrow J^i \cos px \qquad \text{with } J^i \text{ constant}$$

and by translation invariance assume the response of $\langle \phi_y^i \rangle$ is of the same momentum and phase, i.e.

$$\delta \langle \phi_x^i \rangle = \delta \langle \phi_p^i \rangle \cos px \tag{2.25}$$

$$\delta h_x^i = \delta h_p^i \cos px$$

Self-consistency then requires

$$\langle \phi_x^i \phi_x^j \rangle_c \, \delta h_p^j = \frac{\delta \langle \phi_x^i \rangle}{\delta h_x^j} \, \delta h_p^j = \delta \langle \phi_p^i \rangle \tag{2.26}$$

Using the result

$$\cos[p(x+1)] + \cos[p(x-1)] = (2 - p^2) \cos px + O(p^4) \ldots$$

an expression is obtained for the sum in equation (2.24) as $p^2 \rightarrow 0$:

$$\delta h_x^i = (2d - p^2) \, \delta \langle \phi_x^i \rangle + J_x^i \tag{2.27}$$

and substituting (2.27) into (2.26) we have :

$$\delta \langle \phi_p^i \rangle = \langle \phi_x^i \phi_x^j \rangle_c \, [\beta(2d - p^2) \, \delta \langle \phi_p^j \rangle + J^j] \tag{2.28}$$

$$\Longrightarrow \quad [\, p^2 \delta_{ij} + M_{ij}^2 \,] \, \delta \langle \phi_p^j \rangle = \beta^{-1} J^i \tag{2.29}$$

a free-particle wave equation with mass matrix

$$M_{ij}^2 = (\beta \langle \phi_x^i \phi_x^j \rangle_c)^{-1} - 2d \, \delta_{ij}$$

= constant with sources set to zero.

Since at most one component σ_x of ϕ_x has a non-zero expectation value, $<\phi_x^i \phi_x^j>$ is always diagonal.

(i) Symmetric phase

$<\phi_x^i \phi_x^j> \alpha \delta_{ij}$ and there are n degenerate scalars giving masses μ^2:

$$\mu^2 = [\beta <\phi_x^i \phi_x^i>_c]^{-1} - 2d \quad \text{for all } i \qquad 2.30$$

(ii) Broken symmetry

$$<\sigma_x \sigma_x>_c \neq <\pi_x^i \pi_x^j>_c \alpha \delta_{ij} \qquad i,j = 1, \ldots, n-1 .$$

We have one massive scalar

$$\mu_\sigma^2 = [\beta <\sigma_x \sigma_x>_c]^{-1} - 2d \qquad 2.31$$

and it can be shown in accordance with Goldstone's theorem that there are $n-1$ massless Goldstone bosons (see Chapter one)

$$\mu_\pi^2 = [\beta <\pi_x^i \pi_x^i>_c]^{-1} - 2d = 0 \qquad 2.32$$

$i = 1, \ldots, n-1$.

The expectation values $<\phi\phi>$ used in calculating these masses are obtained simply as derivations with respect to h of the expressions obtained for $<\phi>$ earlier in this section.

7 Monte Carlo method and results.

In this section we discuss the evaluation of various expectation values $< Q >$ on a lattice by Monte Carlo methods of integration on a computer.

Recent work by Creutz and others [15,16] has indicated that encouraging results may be obtained even from very small lattices.

Method For this chapter we have used only the standard method of Metropolis [17]. This general algorithm requires only that we know how to generate elements uniformly distributed over our group space - the relevant Boltzmann weight $\exp\{-S\}$ is incorporated for us in the algorithm. In the case of $O(n)$ this means n-component vectors of unit length distributed uniformly on the surface of an n-dimensional sphere. Consider the following method :

Generate $\phi^1, \phi^2, \ldots, \phi^n$ independently each with a Gaussian distribution i.e. $P(\phi^i) \sim e^{-(\phi^i)^2}$, then as the ϕ^i are all independent the combined distribution function $P(\phi)$ is just the product of the $P(\phi^i)$. So $P(\phi) \sim e^{-\sum_i (\phi^i)^2}$, which is rotationally invariant and so constant on the sphere after normalization of ϕ.

In practice however, to speed up computations the spins are chosen with a certain bias. Consider a single site update, and the probability $B(\phi, \phi')$ of selecting a new spin ϕ' for comparison with the old spin ϕ. Then it can be shown that 'detailed balance' requires (see Chapter one)

$$B(\phi, \phi') = B(\phi', \phi) \qquad 2.33$$

In the bias we choose ϕ' close to ϕ, and satisfying (2.33) as follows :

Select N^i from a Gaussian distribution and add to each component ϕ^i of ϕ :

$$\phi^i \rightarrow \phi^i + \varepsilon N^i \qquad 2.34$$

where ε is adjusted 'empirically' to achieve a suitable acceptance rate for the new spins (usually $\gtrsim$ 50%). Vectors generated in this way are distributed'spherically'in an area* above ϕ on the unit sphere. The projection of this area onto the unit sphere forms a uniform distribution in the vicinity of ϕ. Thus after normalization the generated vectors are the ϕ', and since any vector is equally likely, the selection of any ϕ' from any given ϕ is equally likely. Hence (2.33) is satisfied.

Errors

Having written a program to evaluate $< Q >$, we first check the code itself. Comparisons are made to low and high temperature expansions and also to any published results. Standard 5% error bars are given.

It is also important that the samples of configurations used in the sum for $< Q >$ are not statistically correlated in some unnatural way dependent on the updating algorithm. The simplest way to avoid this effect is to take samples only every few updates of the lattice, although more sophisticated methods have been devised [18].

Results

The results of computer simulations are useful with varying reliability for

a) Locating critical points of the system.

b) Establishing the order of a transition and perhaps critical exponents.

c) Extracting correlation lengths near the critical points.

* the size of which depends on ε

(i) $\underline{E(\beta) = \langle \phi_{x+\mu} \phi_x \rangle}$

Rough estimates for (a), (b) are commonly made using $E(\beta)$ [15]. Iterating from either hot or cold starting configurations at fixed β, a phase transition is expected to show up as a slow convergence to equilibrium from the different starts. It is thought that for a first-order transition at β_c, the two starting configurations never converge [19], while for higher-order transitions the two agree if enough iterations are carried out.

Figs. 1a, 1b show $E(\beta)$ for $O(4)$, $d = 4$ with the 'hysterisis loop' around β_c but eventual convergence after many iterations.

(ii) $\underline{M = \langle | \phi_x | \rangle}$

On small lattices it is not easy to establish a spontaneous magnetization at β_c. Fig. 2. shows $M \neq 0$ for all β due to finite size effects.

(iii) $\underline{\chi(\beta) = \frac{1}{N_S}(\langle \sum_{y \neq x} \phi_y \phi_x \rangle - \langle \phi_x \rangle^2)}$

The susceptibility, as defined in section 3 has been used with some success for (b). Tobochnik and Chester [16] consider the $O(2)$, $d = 2$ system. In this case M is always zero (large lattice limit) and χ diverges for all $\beta \geq \beta_c$. In two dimensions large lattices are computationally feasible. Tobochnik and Chester consider lattices up to 60^2 and find evidence for an exponential divergence ('Kosterlitz - Thouless' transition [20]) in ξ as β approaches β_c from above.

For $d = 4$, large lattices are out. The divergence may still be studied, however, by comparing the height and position of the peak in χ for different small lattices (typically 4, 5, 6). This argument is used seriously in Chapter three.

Fig. 3 shows the shift in the peak of χ with lattice size for $O(4)$, $d = 4$, although no attempt is made to extract the power law divergence of the second-order transition.

(iv) $C_v(\beta) = {}^1/N_\ell(\langle [\sum_{x,\mu} \phi_{x+\mu}\phi_x]^2 \rangle - \langle \sum_{x,\mu} \phi_{x+\mu}\phi_x \rangle^2)$

The specific heat C_v is a measure of energy - energy fluctuations and may diverge with χ for a given system as indicated by various scaling relations [9] eg.

$$\alpha = 2 - \nu d$$

where α is the critical exponent of C_v and ν the exponent of ξ.

The system $O(4)$, $d = 4$ (Fig. 4) shows a strong increase in C_v near β_c in contrast to the $d = 2$, $O(2)$ and $O(3)$ cases.

$$C_v = \frac{\partial}{\partial \beta} E(\beta) \qquad 2.35$$

so that measurements of the specific heat may be made from careful analysis of the average energy curve (see Chapter three)

(v) $C(r,\beta) = \langle \phi_{x+r}\phi_x \rangle - \langle \phi_x \rangle^2$

Extracting correlation lengths ξ and hence masses on a computer has proved difficult in practice [21]. Due to the exponential fall off with r, even at distances as small as 3 or 4 $C(r, \beta)$ is small enough to be insignificant compared to the statistical 'noise' of the simulation.

A modification of $C(r, \beta)$ may be used to improve statistics. In addition, the resulting quantity behaves as a pure exponential - it is not modified by the power of r in (2.8).

(vi) $\underline{C'(r,\beta) = \int d^{d-1}\underline{x}\, C(r,\beta)}$

- where integration is over all x directions except the r direction.

Consider $\langle \phi_{x+r} \cdot \phi_x \rangle$ of $C(r,\beta)$. In a field theoretic notation we write

$$\langle \phi_{x+r} \cdot \phi_x \rangle = \langle \phi_{(\underline{x},t)} \cdot \phi_{(\underline{y},0)} \rangle \qquad 2.36$$

where $x_\mu = (\underline{x},t)$ ~

In momentum space we have the small p_μ behaviour

$$\langle \phi_{p_\mu} \cdot \phi_{-p_\mu} \rangle \sim \frac{1}{p_\mu^2 + M^2} \qquad p_\mu = (E, \underline{p})$$

and so we can write

$$\langle \phi_{(\underline{x},t)} \cdot \phi_{(\underline{y},0)} \rangle = \int \frac{d^{d-1}\underline{p}}{(2\pi)^d} \frac{e^{i[Et + (\underline{x}-\underline{y})\cdot p]}}{E^2 + \underline{p}^2 + M^2} \; . \qquad 2.37$$

Integration over $\underline{x}, \underline{y}$ and shifting $\underline{x} \to \underline{x} + \underline{y}$ gives :

$$C'(t,\beta) = \int d^{d-1}\underline{x}\; d^{d-1}\underline{y} \; \langle \phi_{(x.t)} \cdot \phi_{(y,0)} \rangle$$

$$\alpha \int d^{d-1}\underline{x} \int \frac{d^{d-1}\underline{p}}{(2\pi)^d} dE \; \frac{e^{i[Et + \underline{x}\cdot\underline{p}]}}{E^2 + \underline{p}^2 + M^2} \qquad 2.38$$

The $\underline{x}$ integration then may be written as a delta function on $\underline{p}$, and performing the integral over $\underline{p}$ leaves :

$$C'(t,\beta) \; \alpha \int \frac{dE}{2\pi} \frac{e^{iEt}}{E^2+M^2} = \frac{e^{-Mt}}{2M} \qquad 2.39$$

On the Euclidean lattice the time direction is lost and we measure correlations between spins separated by spacial distance r. In Fig. 5 $C(r)$ and $C'(r)$ are compared for the system $O(4)$ with $d = 2$ on an

8^2 lattice. Figs. 6a, 6b show C(r) and C'(r) respectively for O(4) on a 6^4 lattice. Various values of β are considered in the symmetric region - the flattening of the slope as β is increased shows the increasing correlation length as the critical temperature is approached.

For larger distances then, this data shows the advantage of C'(r) over C(r) for measuring correlation lengths. Measuring C(r), up to ten times as many sweeps of the lattice were required to reproduce the straight line of C'(r) fig. 5. Note however that summing over planes for C'(r) requires more work on a computer than C(r), thus the advantages of measuring C'(r) must be weighed against the efficiency of the program.

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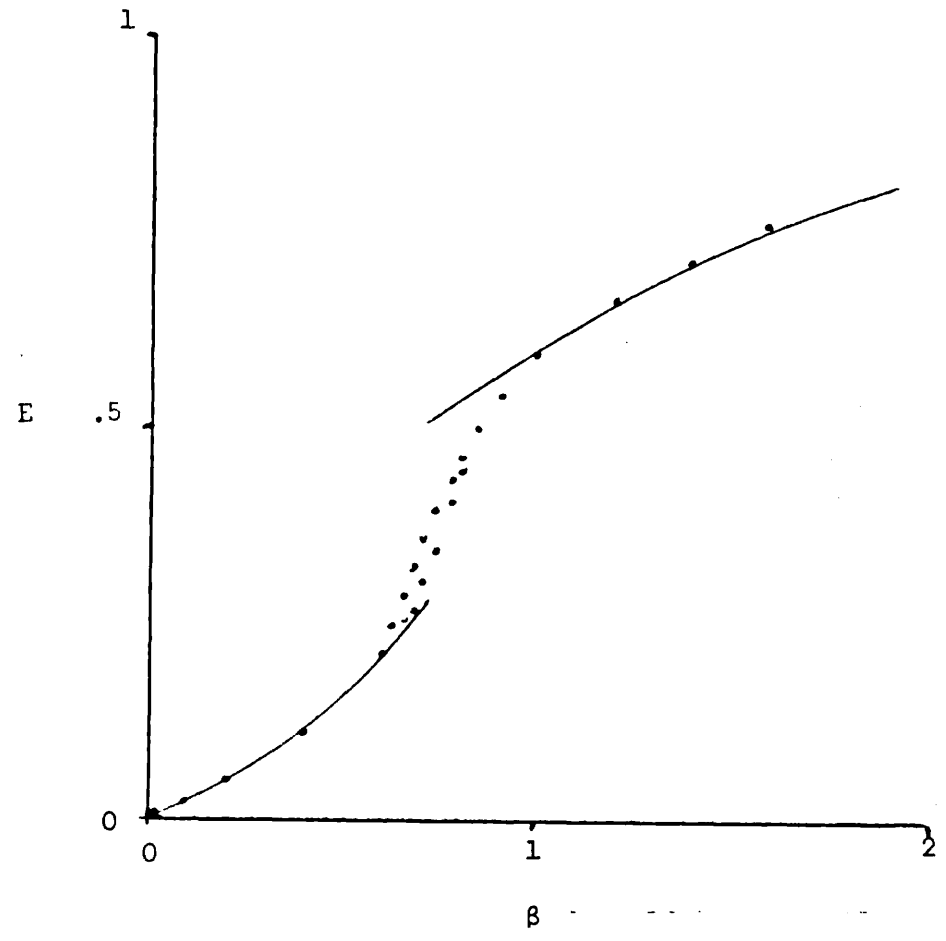

Fig. 1a Average energy $E(\beta)$ for the system $O(4)$ in $d = 4$ on a 6^4 lattice. 30 iterations are made for each data point, averaging only over the last 20 so that thermal equilibrium may be reached. Considerably more than 10 iterations are required to reach equilibrium near the critical point $\beta \underset{\sim}{\sim} .6$. Here, poor convergence from ordered and disordered starting configurations shows up as a 'hysterisis loop' in the thermal cycle between low and high temperatures.

High and low temperature expansions are given.

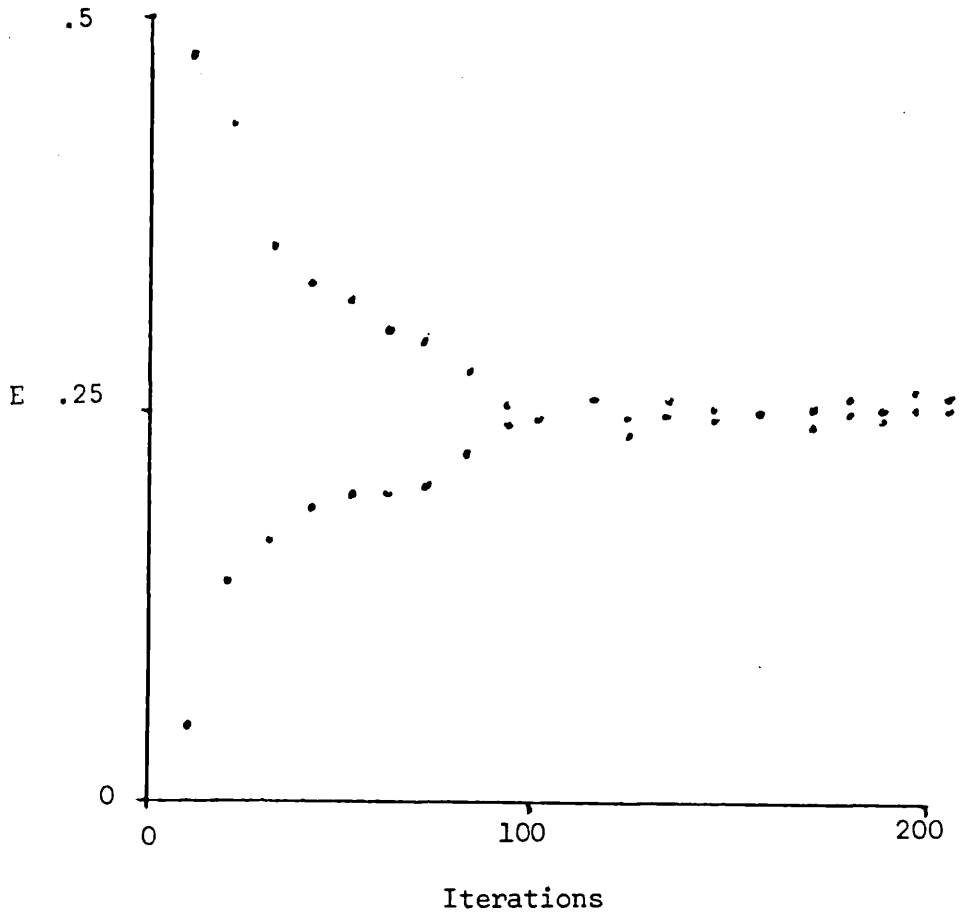

Fig. 1b $E(\beta)$ for the above system at $\beta = .6$. Some convergence is seen to occur after about 100 iterations. 5% error bars would be as small as the data points after $\sim$100 iterations.

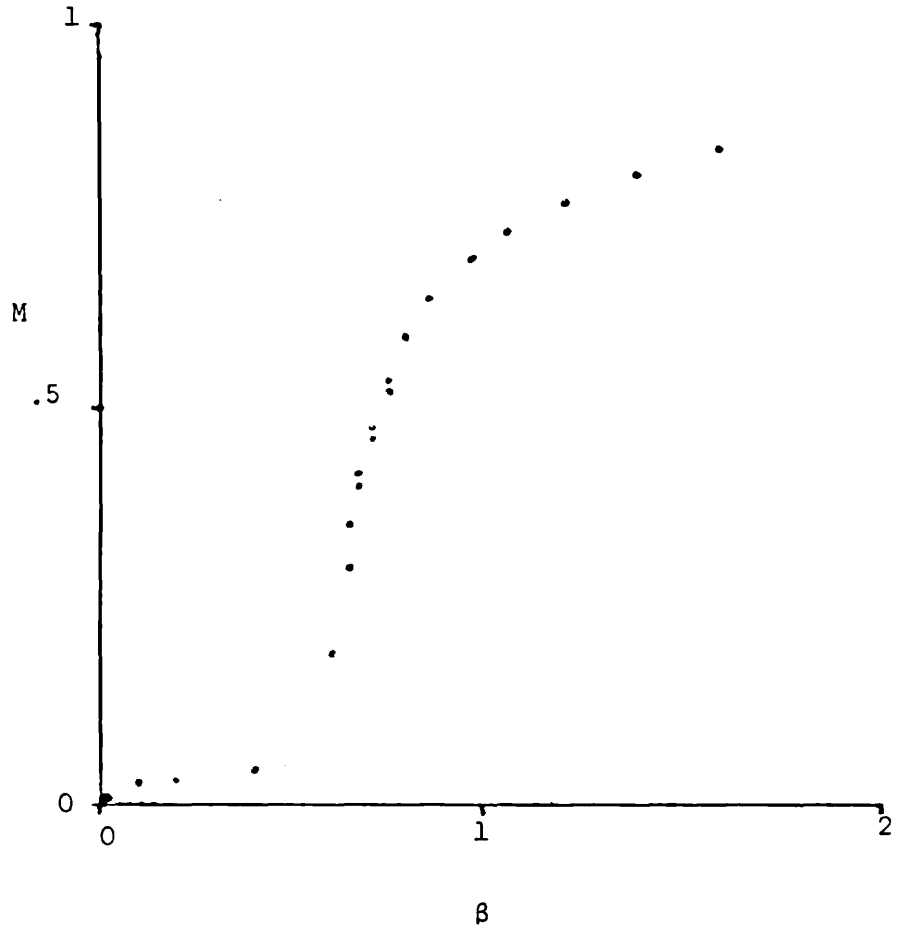

Fig. 2 The Magnetization M for the above system as a function of β.

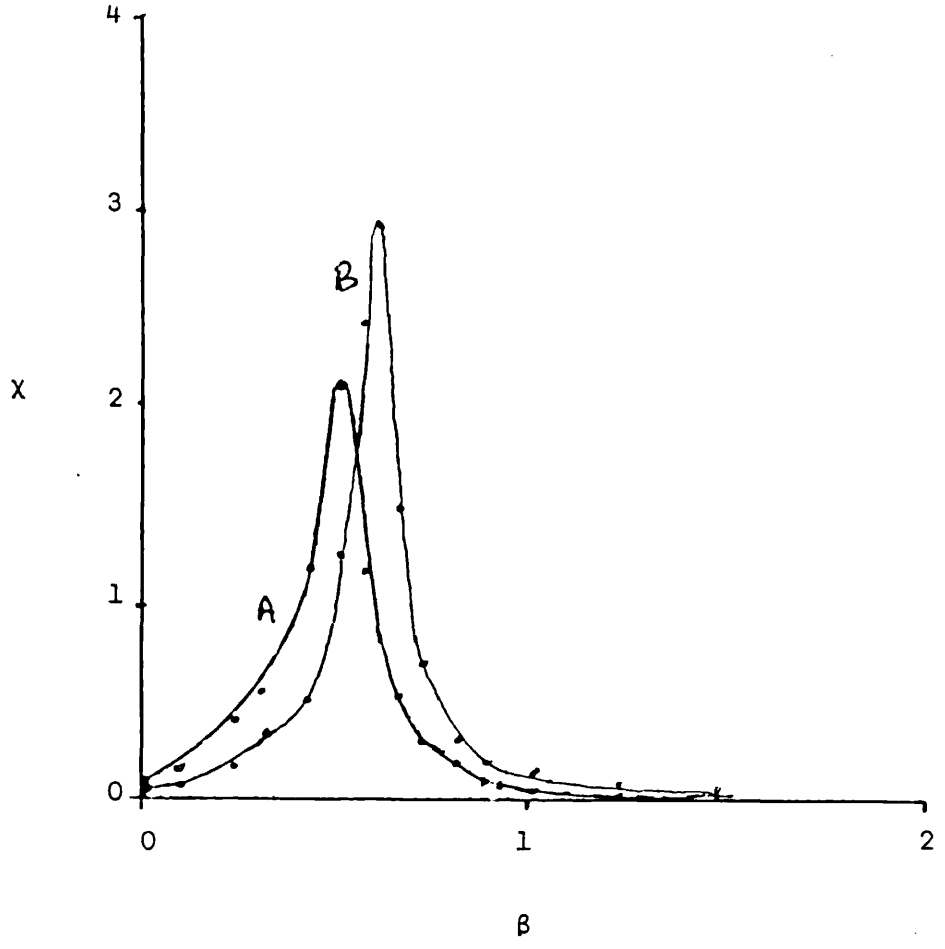

Fig. 3 The susceptibility χ as a function of β.
300 iterations of the whole lattice were made per point, averaging over the last 200 every 3 iterations to avoid correlations between successive updates.
Curves A and B refer to the O(4) system in $d = 4$ for 4^4 and 6^4 lattices. The limited number of data points show some evidence for a shift in χ with lattice size, suggesting a second order transition.

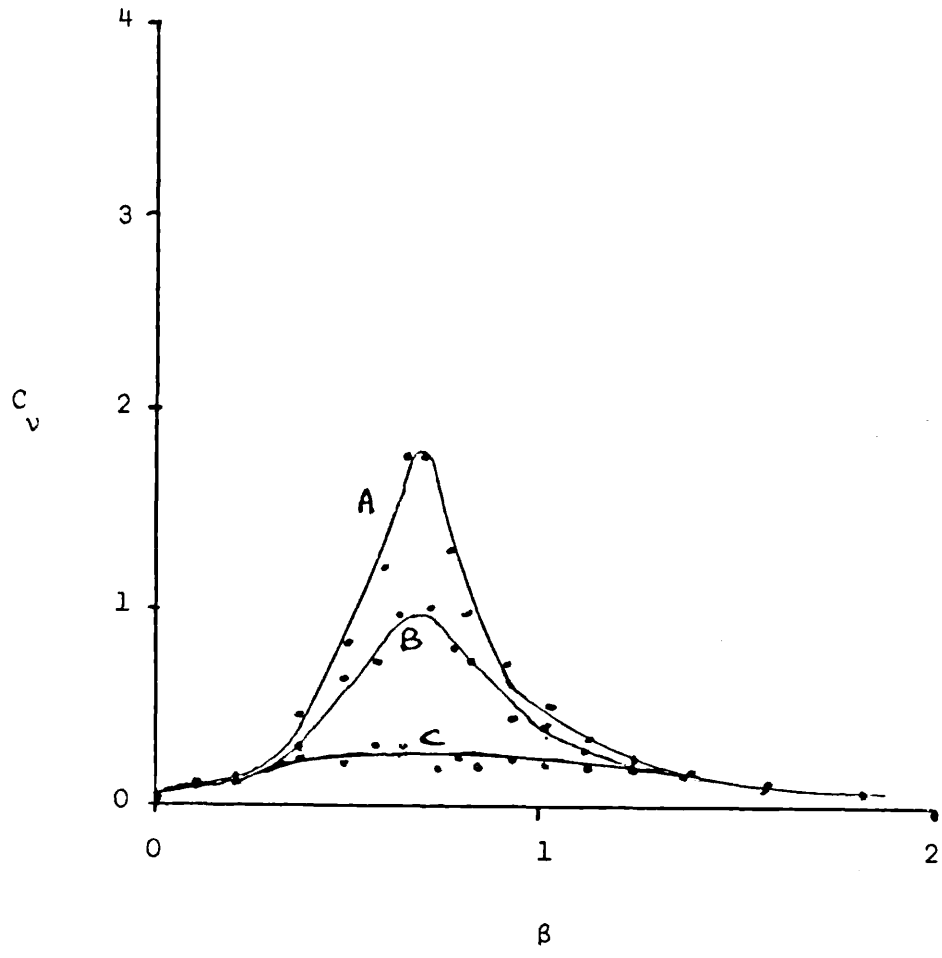

Fig. 4 The specific heat C_v as a function of β.
In the $O(4)$, $d = 4$ case curve A shows C_v diverging with χ. This contrasts with $O(2)$ (curve B) and $O(3)$ (curve C) in $d = 2$ (40^2 lattices used here) these results are consistent with scaling relations.

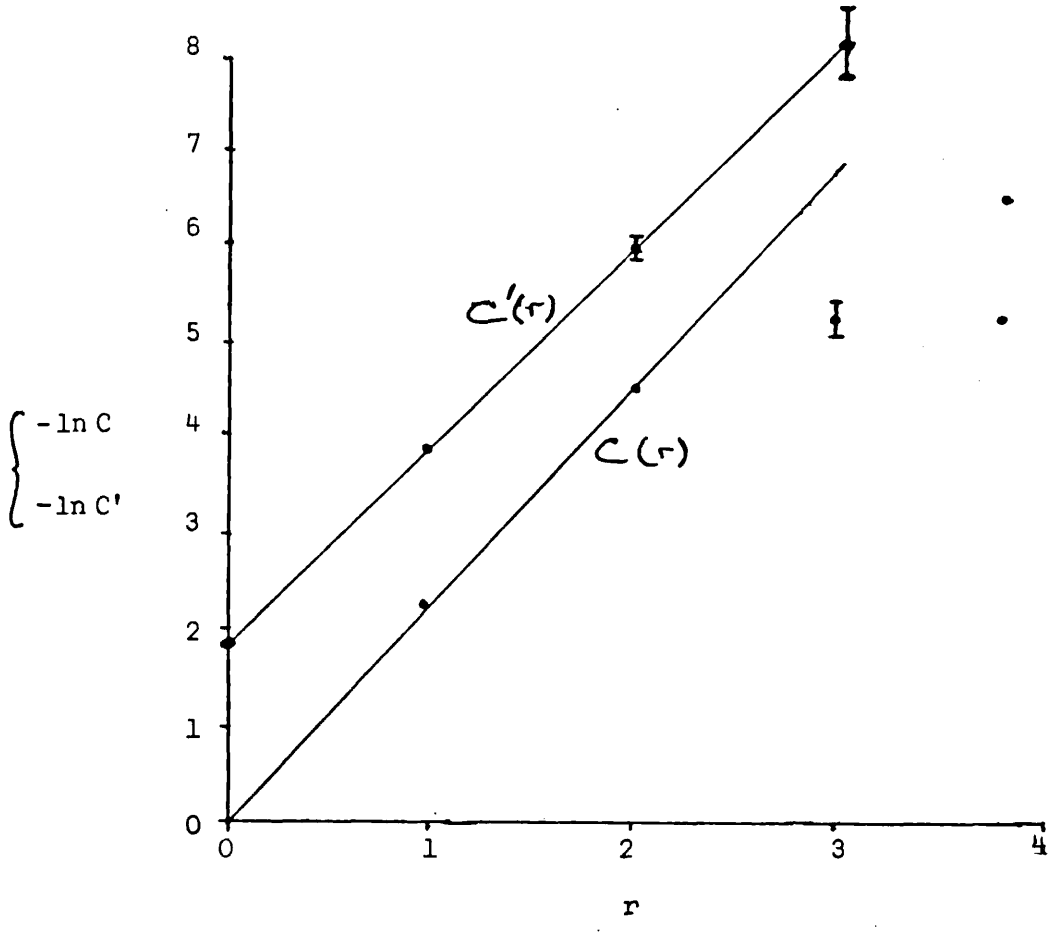

Fig. 5 Comparison of C(r) with C'(r) in the O(4),d = 2 system on an 8^2 lattice in the symmetric region at $\beta = .4$.
Taking -lnC extracts the correlation length. 300 iterations were made, averaging over the last 200 every 3 updates.
5% error bars are given where they are not smaller than the data points.
On a finite lattice we may only measure correlations between spins separated by distances less than the lattice size, since at larger distances the periodicity of the lattice introduces extra correlations. Hence correlations are measured here only up to $r = 3$. At $r = 3$ C'(r) compares favourably with C(r), although at $r \leq 2$ results are similar.

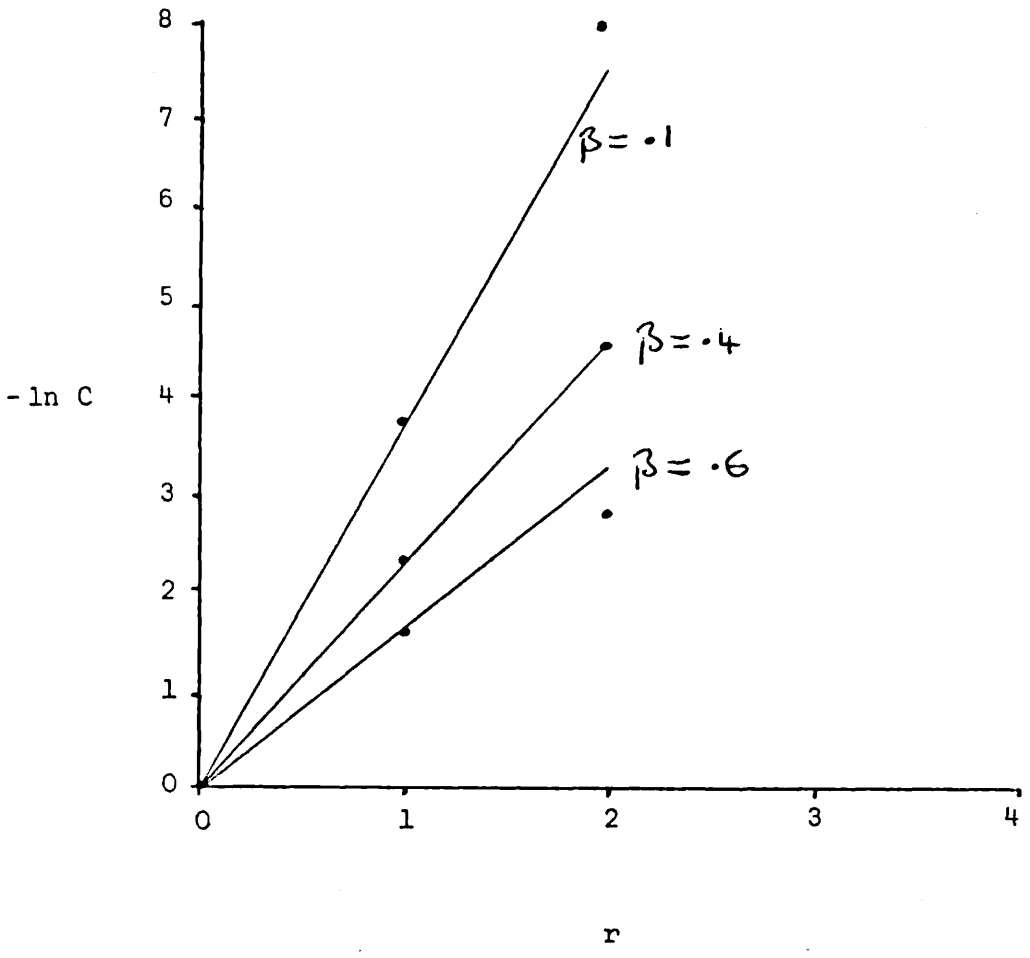

Fig. 6a Increasing correlation lengths with β, extracted from $C(r)$ in the symmetric phase of $O(4)$ in $d = 4$ on a 6^4 lattice. Errors are as small as the data points after 200 iterations.

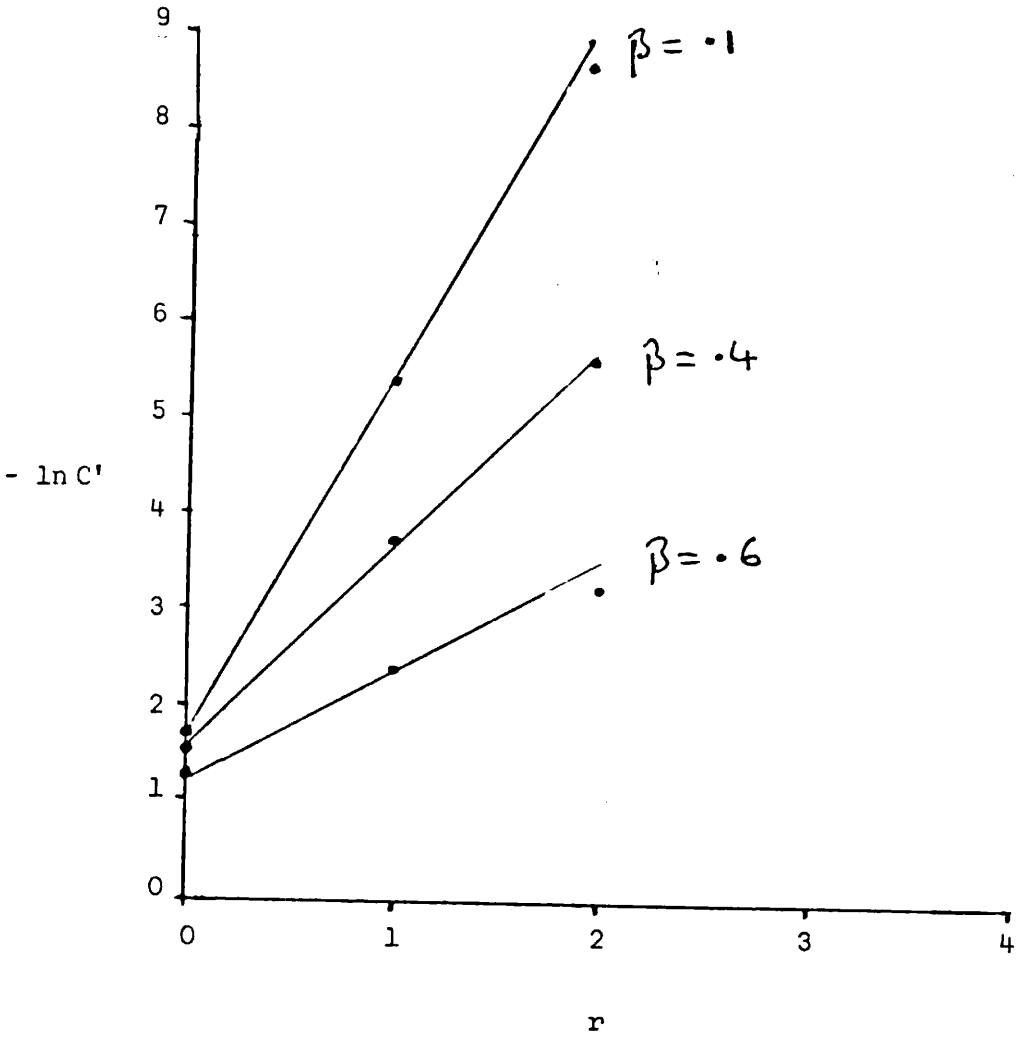

Fig 6b As for fig. 6a but with C'(r). No improvement on C(r) is found on this smaller lattice.

PURE GAUGE THEORY

CHAPTER 3

In this chapter we firstly review some properties of another limit of the mixed model - pure U(1) lattice gauge theory in four dimensions. These results are compared with a computer simulation of four dimensional SU(3) gauge theory.

If we are to follow the example of the spin models and search for a characteristic length ξ in a gauge system, then we are restricted by Elitzur's theorem [1] to measurements between gauge invariant objects. Since the average field $< U_x^\mu >$ vanishes in a gauge theory there can be no direct analogy of the susceptibility χ [i.e. field-field correlations] of Chapter two.

Recall that the simplest gauge invariant objects on the lattice are plaquettes. We might hope that a measurement of correlations between distant plaquettes could reveal some kind of phase structure familiar in spin models. To this end we differentiate the average action equation 1.10, giving the gauge analogue of χ, the specific heat C_ν :

$$C_\nu = \frac{\partial}{\partial \alpha} E(\alpha)$$

$$= < \sum_{\square \neq \blacksquare} U_{\square} \cdot U_{\blacksquare} > - < U >^2 \qquad 3.1$$

and so contributions from distant plaquettes to (3.1) will show up in C_ν near second-order phase transitions.

The abelian case

1. Definition

Consider the Wilson action from Chapter one for $U(1)$ with elements U_x^μ residing on the links of a four-dimensional lattice:

$$U_x^\mu = e^{iea\theta_x^\mu}$$

$$(U_x^\mu)^{-1} = U_{x+\mu}^{-\mu} = e^{-iea\theta_x^\mu} \qquad 3.2$$

where $0 \leq \theta_x^\mu \leq {}^{2\pi}/_{ea}$

and e is the conventional bare coupling constant of a field theory.

The sum over all plaquettes is then the action:

$$S_{U(1)} = \sum_{x,\mu\nu} \mathrm{Tr}\, \frac{1}{2} [U_x^\mu\, U_{x+\mu}^\nu\, U_{x+\mu+\nu}^{-\mu}\, U_{x+\nu}^{-\nu} + \mathrm{h.c}]$$

$$= \sum_{x,\mu\nu} \cos\{ea[\theta_x^\mu + \theta_{x+\mu}^\nu - \theta_{x+\nu}^\mu - \theta_x^\nu]\} \qquad 3.3$$

(3.3) is invariant under local transformations $e^{i\psi_x}$, $e^{-i\chi_{x+\mu}}$ on the sites

$$e^{iae} \to e^{i\psi_x}\, e^{iae\theta_x^\mu}\, e^{-i\chi_{x+\mu}}$$

$$S_{U(1)} \to S_{U(1)} \qquad 3.4$$

Integration over all links defines the partition function:

$$Z(\alpha) = \int \prod_{x,\mu} D\, U_x^\mu \exp\{\alpha\, S_{U(1)}\} \qquad 3.5$$

where α will be related to e.

The normalized measure $D\,U_x^\mu$ for $U(1)$ is simply $DU_x^\mu = \frac{1}{2\pi}\, D\theta_x^\mu$ and averages over $U(1)$ invariant qualities $Q_{U(1)}$ are:

$$\langle Q_{U(1)} \rangle = Z^{-1} \int \prod_{x,\mu} D\theta_x^\mu \, Q_{U(1)} \exp\{\alpha S_{U(1)}\} \qquad 3.6$$

2. High and low α

Expansions similar to those for the spin models are discussed in appendix B. For large α (low temperature) a 'gauge fixing' term needs to be introduced into the action as with continuum perturbation theories. At small momentum p, i.e. long wavelengths, where the lattice spacing becomes unimportant, the low temperature result reduces to that of continuum electrodynamics.

The results for the average energy density (average plaquette) E_p are compared with Monte Carlo data in fig. 1 for $d = 4$.

(i) High α

$$E_p \simeq \frac{\alpha}{2} - \frac{\alpha^3}{16} + \frac{13}{96}\alpha^5 + O(\alpha^7) \ldots \qquad 3.7$$

(ii) Low α

$$E_p \simeq 1 - \frac{1}{4\alpha} - \frac{1}{32}\alpha^2 + O(\alpha^{-3}) \ldots \qquad 3.8$$

3. Naive continuum limit

In parallel with spin systems in two dimensions, lattice gauge theories reduce in the limit $a \to 0$ to the desired continuum form only if $d = 4$.

For U(1), obtaining this limit is a very swift exercise:

Writing the product of U_x^μ's round a plaquette of equation 3.3 as $U_\square$, we use a suggestive notation:

$$U_\square = \exp[iea^2 F_{\mu\nu}] \qquad 3.9$$

where $$F_{\mu\nu} = \Delta_\mu \theta_x^\nu - \Delta_\nu \theta_x^\mu$$

and $\Delta_\mu \theta^\nu_x := (\theta^\nu_{x+\mu} - \theta^\nu_x)/a$

approximates a derivative.

The real part of $U_\square$ gives

$$\text{Re } U_\square = \cos[ea^2 F_{\mu\nu}]$$

$$\simeq \frac{e^2 a^4}{2} F^2_{\mu\nu} + \ldots \qquad 3.10$$

Replacing $\sum_{x,\mu\nu}$ in (3.2) by $a^{-4}\int d^4x$ and taking $a \to 0$ leaves

$$S_{U(1)} \underset{a\to 0}{\to} \frac{e^2}{2}\int d^4x\, F^2_{\mu\nu} \qquad 3.11$$

We recognise here the conventional Yang-Mills action for electrodynamics. e^2 is absorbed into the definition of α in (3.5), thus we have for this model:

$$\alpha = \frac{1}{e^2} \qquad 3.12$$

4. The second-order transition

As discussed in Chapter one, the $U(1)$ gauge theory in four dimensions is known to undergo a transition at finite coupling [2] Experience with spin models has given rise to two main views on the nature of this transition. On one hand an analogy is made with the two dimensional $O(2)$ spin model (in accordance with the Migdal-Kadanoff recursion relations). The correlation length here is expected to diverge exponentially near the critical point [3]:

$$\xi \underset{T\to T_c^+}{\sim} \exp\{b\,(\frac{T_c}{T-T_c})^{\frac{1}{2}}\} \qquad 3.13$$

This has been explained in terms of the unbinding of vortices

beyond the critical temperature [4]. The analogy in four dimensions is seen as the unbinding of monopole strings [5], and this has been observed in a computer study by Degrand and Toussaint [6].

However, there has appeared much evidence from Monte Carlo simulations supporting the existence of a conventional power law divergence (second-order transition) of the gauge theory at the critical region [7 , 8 , 9]

$$\xi \sim |T - T_c|^{-\nu} \qquad 3.14$$

A renormalization group analysis carried out by Hamber [10] also supports this view.

We consider here an approach very similar to that of Lautrup and Nauenberg [7], using Monte Carlo simulation on small lattices together with a finite size scaling method*† [11] :

Consider the correlation length $\xi_L(T)$ for a finite lattice of size L^d . Then by definition $\xi_L \leq L$ and we write

$$\xi_L = L\,S(x) \qquad 3.15$$

where S is a scaling function to be determined. x is a variable characteristic of the system. It is convenient to choose :

$$x = |T - T_L|\, L^{1/\nu} \qquad 3.16$$

where T_L is the critical temperature of the finite system.

Some simple properties of S follow :

* See ref.[8] for a slightly different use of this method to extract the critical index ν.

† The validity of this approach has been called into question, however [12] .

1) Clearly $S(0) = 1$ 3.17

since $\xi_L = L$ at $T = T_L$

2) Up to a certain distance T_ε from T_c we might expect the finite system to mimic the infinite one, i.e.

$$\xi_L \sim |T - T_L|^{-\nu} \qquad 3.18$$

for $|T - T_L| \geq T_\varepsilon$

For $|T - T_L| < T_\varepsilon$ (3.17) and (3.18) would be inconsistent.
Equation 3.18 is obtained by assuming the asymptotic behaviour:

$$S(x) \sim x^{-\nu} \qquad 3.19$$

for $x \to \infty$.

3) Obtaining ξ_L for T very close to T_L then amounts to making corrections to (3.19) for $|T - T_L| < T_\varepsilon$ consistent with (3.17).
A simple choice is:

$$S(x) = (1 + \lambda x^2)^{-\nu/2} \qquad 3.20$$

with λ a free parameter.

We are now in a position to estimate the critical behaviour of the system. Consider the large L behaviour

$$\xi \simeq \xi_L$$

$$\Rightarrow \quad |T - T_c|^{-\nu} \simeq L\,S(x) \qquad 3.21$$

In particular, for $T = T_L$, using (3.17)

$$\Rightarrow \quad |T_L - T_c|^{-\nu} \simeq L \qquad 3.22$$

Experience shows that $T_L > T_c$ for all finite L and so

$$T_L - T_c \sim L^{-1/\nu} \qquad 3.23$$

Now take the specific heat

$$C_v \sim |T - T_c|^{-\alpha} \qquad 3.24$$

Using the relation $\alpha = 2 - \nu d$ [13] we have

$$C_L(T = T_L) \sim |T_L - T_c|^{-\alpha}$$

$$= [|T_L - T_c|^{-\nu}]^{2/\nu - d}$$

$$= L^{2/\nu - d} \qquad 3.25$$

from (3.22).

In ref. [7] T_L is found using Monte Carlo simulation for the ('normalised') specific heat with $L = 4,5,6$. The scaling function of (3.20) with $\lambda = 0.6$ is then used to obtain a fit to the data for C_L. Good fits are claimed when $\nu = \frac{1}{3}$. T_c is estimated from (3.23) so that the parameters used to fit C_L may be used to estimate C_L in the limit $L \to \infty$.

In the next section we assume a value for T_c and consider lattice sizes 4,5,6. Equation 3.23 is then used to estimate ν. For comparison, an independent estimate for ν is made using (3.25).

5. Monte Carlo results

The convergence of Monte Carlo data in the neighbourhood of a second-order transition is in general very slow [14], indeed this is

often taken to be the signal for such a transition.

The 'heat bath' algorithm of Creutz has been extensively used [14,15,16,17] to speed up computations. Implementation of this method, however is technically more difficult [see Introduction]. In appendix B the simple case of U(1) is compared with the algorithm for SU(3).

Results

As many as 6000 updates of the whole lattice were made in order to obtain equilibrium data in the critical region. In addition, many data points were required to be sure of locating the peaks in C_L.

Fig. 1 shows $E(\alpha)$ for $L = 6$. The error bars are smaller than the data points.

The results for T_L and C_L are :

		$T_L (= 1/\alpha_L)$	C_L
	4	1.02	3.43
L	5	1.005	5.50
	6	.996	7.98

With this limited data we are able to estimate the constant of proportionality in (3.23) and (3.25) and the critical exponent ν. Both (3.23) and (3.25) yield estimates of ν that are consistent with $\nu = \frac{1}{3}$ ($\sim .25$ and $\sim .32$ respectively) although the result for (3.23) is a little small.

An attempt was also made to measure correlations between plaquettes

separated by distance r. Unfortunately, the results were statistically insignificant for $r > 1$.

6. Remarks

We have presented evidence for a second-order phase transition in the infinite system at $\alpha = .998$. It is known from exact evaluation of systems with discrete symmetries [18] that lattices as small as $L = 2$ do not indicate the correct large L behaviour. It is hoped however, that the slightly larger lattices considered here are suitable for the finite size scaling analysis. It is encouraging at least that the behaviour of the $U(1)$ system for $L = 4,5,6$ differs from that of $SU(2)$ [19] and the $SU(3)$ case we consider next.

As commented by other authors [8, 9] it may be possible to fit the data to an essential singularity as in the two dimensional $O(2)$ spin model. Larger lattices and better statistics would be required to confirm the algebraic singularity in the specific heat with exponent $\nu \underset{\sim}{\sim} \frac{1}{3}$.

Note that mean field theory predicts a transition at $\alpha \underset{\sim}{\sim} 1$, but indicates incorrectly a first-order transition. Masses may also be extracted in this scheme [20].

The non-abelian case

The properties of SU(3) lattice gauge theory have been discussed in Chapter one - we now make computations for comparison with the U(1) case.

7. The specific heat of SU(3)

Recall the SU(3) lattice action of 1.

$$S_{SU(3)} = \frac{1}{2} \sum_{x,\mu\nu} [T_r(U_x^\mu U_{x+\mu}^\nu U_{x+\mu+\nu}^{-\mu} U_{x+\nu}^{-\nu} + \text{h.c.})] \qquad 3.26$$

where U_x^μ is the SU(3) matrix $\exp [\, iae \sum_{b=1}^{8} \frac{\lambda^b}{2} A_x^{\mu b}]$.

The partition function is

$$Z(\alpha) = \int \prod_{x,\mu} D U_x^\mu \; \exp\{ \alpha S_{SU(3)} \} \qquad 3.27$$

where $\alpha = 6/e^2$.

Writing $U = (\underline{X}, \underline{Y}, \underline{Z})$ where $\underline{X}, \underline{Y}, \underline{Z}$ are 3-vectors, the following SU(3) constraints are imposed on the measure $D U_x^\mu$ in the form of delta functions:

$$\begin{aligned} 1 &= \underline{X}^* \cdot \underline{X} = \underline{Y}^* \cdot \underline{Y} = Z^* \cdot \underline{Z} \\ 0 &= \underline{X}^* \cdot \underline{Y} = \underline{X}^* \cdot \underline{Z} = \underline{Y}^* \cdot \underline{Z} \end{aligned} \qquad 3.28$$

$$\text{Det } U = +1 .$$

A 'heat bath' Monte Carlo simulation was used to measure the specific heat of (3.1) on lattice sizes 4,5,6. The results are shown in fig. 3. They are similar to those found by Lautrup and Nauenberg for SU(2) [19]. There is a peak in the specific heat

at around $\alpha \underset{\sim}{} 6.00$ which does not appear to increase with lattice size, unlike the U(1) case. There is, however, a small shift in the position of the curve.

8. Remarks

The behaviour of the non-abelian system near $\alpha \underset{\sim}{} 6.00$ appears to be of a novel character. If the confinement property at small α is to persist for all values of the coupling, then we would hope that this is not a signal for a change of phase, such as occurs in the abelian system.

The peak occurs near to where Creutz [21] and Pietarinen [17] find a rapid crossover in the string tension from the strong coupling region matching on to the known Q.C.D. behaviour at weak coupling. Since the height of the peak does not increase with lattice size we might hope that correlations are not large in this region. It is not clear why there is a shift in the position of the curve, although this might be related to the onset of asymptotic freedom in the weak coupling region.

The possibility of a 'roughening' transition has been suggested [22]. A roughening transition forms a natural barrier to the extrapolation of strong coupling series for quantities like the string tension. This weak singularity takes the form of fluctuations in the surfaces spanned by Wilson loops and may be measurable even on very small lattices [23]. Such a transition may affect computer simulations by slowing down the approach to equilibrium configurations and by increasing finite size effects. For analytic calculations the problem is more serious in that care may need to be taken in the choice of quantity to be measured if a matching of low to high α is required.

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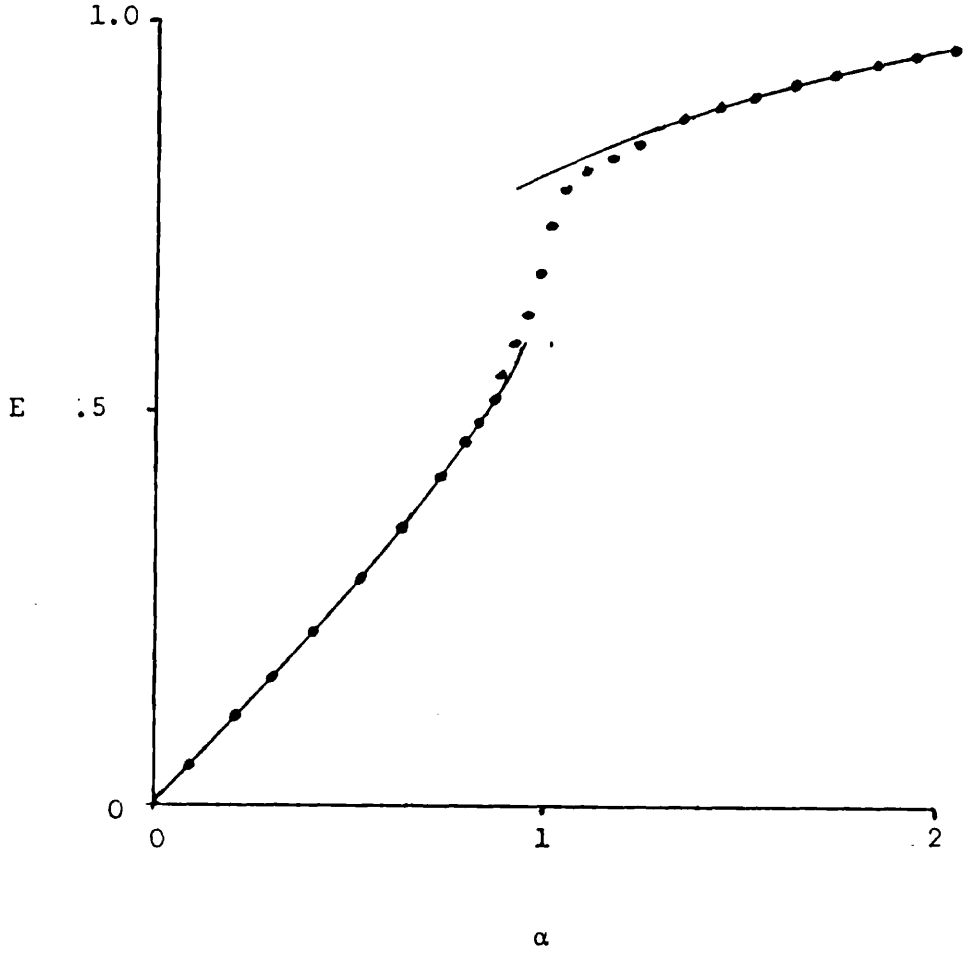

Fig. 1

E versus α for U(1) on a 6^4 lattice. Data points in the critical region are the result of 6000 sweeps of the lattice, averaging over the last 5800 every 3 sweeps. Error bars would be smaller than the points.

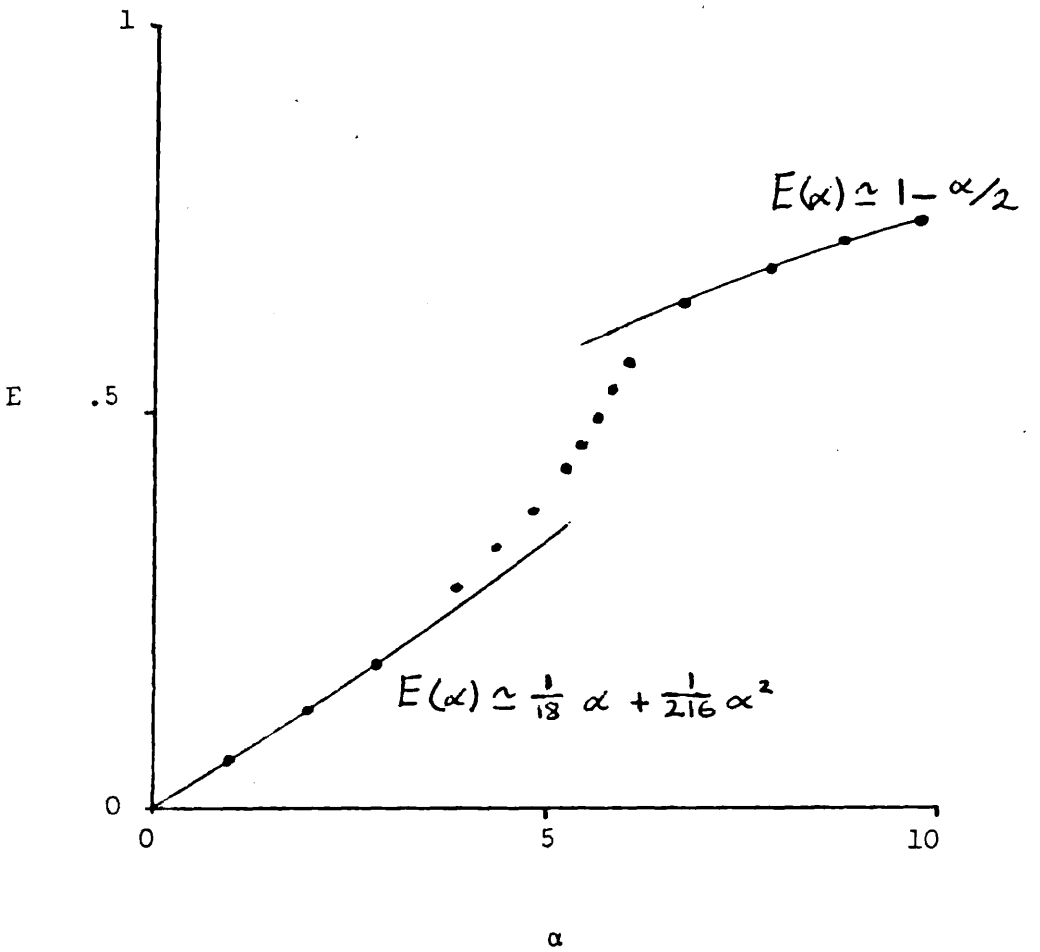

Fig. 2

E versus α for SU(3) on a 5^4 lattice. Statistics are as for fig. 1. High and low α curves are also given.

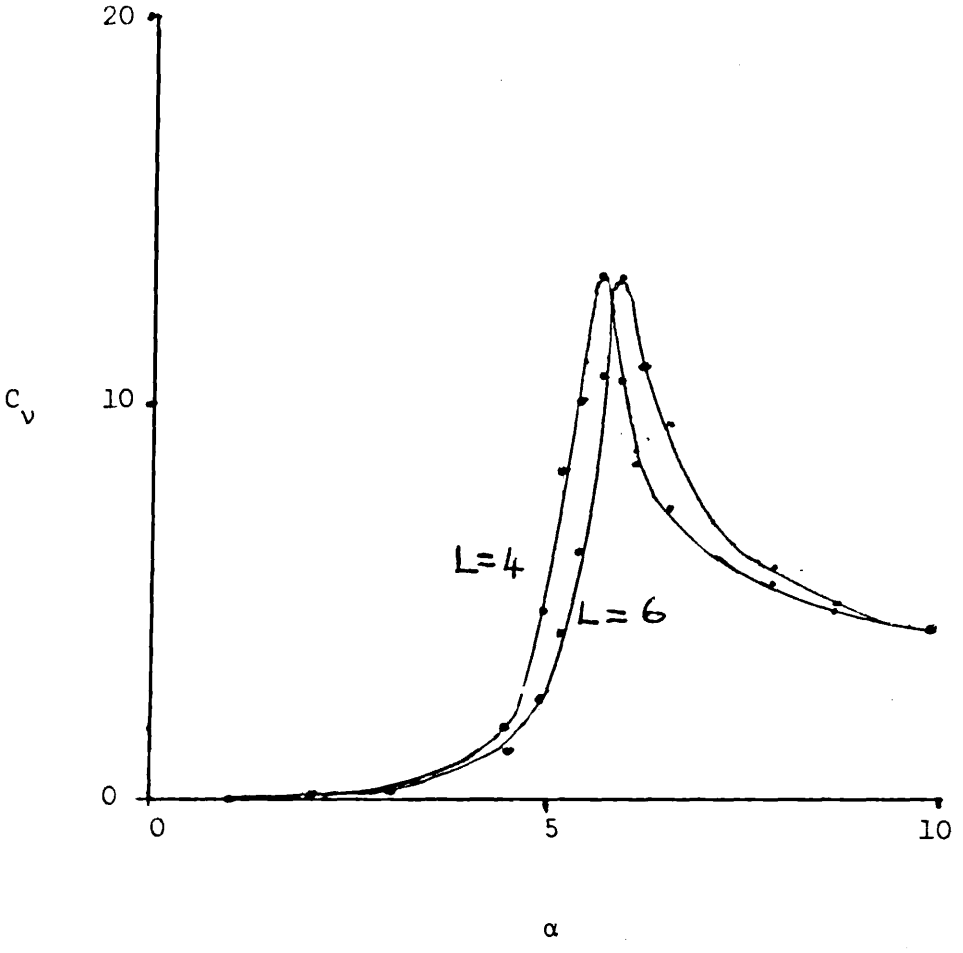

Fig. 3

C_ν versus α for SU(3) in four dimensions, showing the effect of increasing lattice size L. Statistics are as for figs. 1 and 2 with curves fitted by eye.

CHAPTER 4 CP^{n-1} COUPLED TO GAUGE FIELDS.

In this chapter matter (spin) fields are coupled to the pure abelian gauge theory of Chapter three. Various coupled systems have been studied both analytically [1-4] and by Monte Carlo simulations [5-9]. We shall consider the case of U(1) coupled to fixed length scalar (Higgs) fields. More site spins are introduced (each in the fundamental representation of the gauge group) than are needed to break the gauge symmetry completely. Under certain conditions this lattice model reduces in the continuum limit to n-component scalar Q.E.D.*

1. The mixed model

We consider a lattice action of the form :

$$S = \frac{\alpha}{2} \sum_{x,\mu\nu} U_x^{\mu} U_{x+\mu}^{\nu} U_{x+\mu+\nu}^{-\mu} U_{x+\nu}^{-\nu} + \frac{\beta}{2} \sum_{x,\mu} Z_x^a U_x^{\mu} \bar{Z}_{x+\mu}^a + \text{h.c.} \qquad 4.1$$

where Z_x^a is an n-component complex vector satisfying the fixed length condition on each site:

$$\sum_{a=1}^{n} Z_x^a \bar{Z}_x^a = 1 \qquad 4.2$$

The gauge group is U(1) and we have as before :

$$U_x^{\mu} = e^{iaeA_x^{\mu}} \qquad 0 \leq A_x^{\mu} < 2\pi$$

while the matter fields are written

* One motivation for studying this model is to understand the suggested connection between U(1) and CP^{n-1} field theories [18], although work by Callaway and Carson [7] has not lent support to this idea.

$$Z_x^a = (r_x^1 e^{i\theta_x^1}, r_x^2 e^{i\theta_x^2}, \ldots, r_x^n e^{i\theta_x^n})$$

$$0 \leq \theta_x^a < 2\pi \qquad a = 1, \ldots, n$$

Then using previous notation (4.1) becomes

$$S = \alpha \sum_{x,\mu\nu} \cos[aeF_{\mu\nu}] + \beta \, \mathrm{Re} \sum_{x,\mu} Z_x^a \bar{Z}_{x+\mu}^a e^{iaeA_x^\mu} \qquad 4.3$$

The action (4.3) is invariant to the local transformations:

$$\begin{aligned} A_x^\mu &\to A_x^\mu + \Delta_\mu \psi_x \\ \theta_x^a &\to \theta_x^a + \psi_x \end{aligned} \qquad 4.4$$

while the spin fields also lie in the fundamental representation of the global symmetry group $U(n)$.

Making the usual replacements

$$\begin{aligned} \Delta_\mu &\to a\partial_\mu \\ \sum_{x,\mu} &\to a^{-d} \int d^d x \end{aligned} \qquad 4.5$$

and rescaling Z_x^a

$$Z_x^a \to Z_x'^a = a Z_x^a / \sqrt{\beta} \qquad 4.6$$

we obtain the naive continuum limit of (4.3) in four dimensions:

$$S \to \int d^4 x [\tfrac{1}{4} F_{\mu\nu}^2 + \tfrac{1}{2} |(\partial_\mu + ieA_x^\mu) Z_x^a|^2] \qquad 4.7$$

as $a \to 0$.

The constraint (4.2) may be incorporated by allowing $|Z_x^a|$ to fluctuate, but adding a suitable potential term to the action (4.1):

$$S \to S' = S + \lambda \sum_x (\bar{Z}_x^a Z_x^a - 1)^2 \qquad 4.8$$

Then in the limit $\lambda \to \infty$* configurations different from unity are not important. Defining

$$\lambda' := \lambda/\beta^2$$

$$f := \beta/a^2$$

and taking the limit $a \to 0$ as before then gives

$$S' \to \int d^4x \left[\frac{1}{4} F_{\mu\nu}^2 + \frac{1}{2}|(\partial_\mu + ieA_x^\mu) Z_x^a|^2 + \lambda'(|Z_x^a|^2 - f)^2\right] \qquad 4.9$$

- a Euclidean action for n-component scalar Q.E.D.

The partition function is defined as

$$Z(\alpha,\beta) = \int \prod_{x,\mu} D A_x^\mu \prod_x D Z_x^a D \bar{Z}_x^a \, \delta(\bar{Z}_x^a Z_x^a - 1) \exp\{-S\} \qquad 4.10$$

and only gauge-variant quantities will gain non-zero expectation values.

2. Limits of α and β.

The expression (4.10) for Z simplifies in the various extreme limits of α and β.

a) $\beta \to 0$

When $\beta = 0$ the integration over the $Z_x^{a'}s$ is trivial and

* See Discussion (section seven).

the model is reduced to the pure U(1) gauge theory of Chapter three, with a second-order phase transition at $\alpha \underset{\sim}{} 1$ separating the confining and Maxwell phases.

Suppose we consider small but non-zero β. Consideration of strong coupling diagrams indicates the form of these extra interactions. The first contribution will occur when four links lie around a single plaquette, i.e. $O(\beta^4)$. Since this is a 'plaquette term' we may interpret the first correction as an addition to the pure gauge action, i.e. a renormalization of α by $+ \beta^4/8n^3$.

Following this line of reasoning we would expect a line of transitions ending at the pure U(1) theory given by:

$$\alpha_c(\beta) \underset{\sim}{} \alpha_c(0) - \beta^4/8n^3 + O(\beta^6) \ldots \qquad 4.11$$

We expect this line of transitions to be of the same order as the pure gauge theory, although we cannot be sure of the effect of higher order (non-plaquette) modifications.

b) $\beta \to \infty$

Here the configurations that minimize the sum over links in (4.3) have the spins frozen (magnetized).* In addition the link variables are forced into a pure gauge configuration. Hence there is no α dependence and the model is trivial in this limit.

c) $\alpha \to 0$

For $n = 1$ [4] following consideration of a suitable gauge transformation the model is seen to be trivial in this limit. For the cases $n > 1$ that we consider this cannot occur.

* Up to gauge equivalence.

For $\alpha = 0$, the link variables factorize, giving

$$Z(0,\beta) = \int \prod_x D Z_x^a D \bar{Z}_x^a \, \delta(\bar{Z}_x^a Z_x^a - 1) \prod_{x,\mu} \int_0^{2\pi} d\theta \, \exp\{\beta |Z_x^a \bar{Z}_{x+\mu}^a| \cos\theta\} \qquad 4.12$$

$$= \int \prod_x D Z_x^a D \bar{Z}_x^a \, \delta(\bar{Z}^a Z^a - 1) \exp\{ \sum_{x,\mu} \ln I_0(\beta \, | \, Z_x^a \bar{Z}_{x+\mu}^a \, |)\} \qquad 4.13$$

The resulting 'action' of (4.13) may be written in terms of gauge invariant projectors

$$P_x^{ab} = \bar{Z}_x^a Z_x^b \qquad 4.14$$

where $$(P_x^{ab})^2 = P_x^{ab} \qquad 4.15$$

and $$\text{tr } P_x^{ab} = 1$$

Expanding the Bessel function in (4.13) the action reads

$$S_{CP^{n-1}} = \sum_{x,\mu} \ln I_0(|Z_x^a \bar{Z}_{x+\mu}^a \, | \, \beta)$$

$$\sim \sum_{x,\mu} [\beta^2/4 \text{ tr } P_x^{ab} P_{x+\mu}^{ab} - \beta^4/64 (\text{tr } P_x^{ab} P_{x+\mu}^{ab})^2 + \ldots] \qquad 4.16$$

(4.13) now has the form of a lattice CP^{n-1} model [10,11] and might be expected to possess a first-order phase transition except for $n = 2$ and possibly other low values of n [12].

d) $\alpha \to \infty$

In this instance the link variables are 'frozen' into pure gauge configurations. Then the model is 'gauge equivalent' to the O(2n) Heisenberg spin model. We expect the same transitions as we found in Chapter two except that singularities only occur in gauge

invariant objects, and not for example in the average field (magnetization) $< Z_x^a >$.

When α and β are large but finite a perturbation expansion may be made. The matter fields are assumed to be slowly varying about a given direction and a suitable gauge transformation fixes Z_x^a to be real. Then expanding in the gauge field results in the addition of a mass term (in the continuum limit) to the pure U(1) propagator of equation (B 2.4).

3. The phase diagram - Monte Carlo results.

As a guide to the physics of this model we use a computer simulation to map out the phase diagram in the (α,β) plane for $n = 2,3$ on a 4^4 lattice. We use the Metropolis algorithm and by analogy with Chapter two, random numbers selected from a normal distribution are used to update the spins and links with an appropriate bias.

To search for possible phase transitions we consider expectation values of the link and plaquette terms contributing to the action (4.3)*

$$< P > \; = \; \frac{1}{2} < \cos[F_{\mu\nu}] > \qquad 4.17$$

$$< L > \; = \; \frac{1}{2} < Z^a \, e^{iA_x^\mu} \, \bar{Z}^a_{x+\mu} + \text{h.c.} > \qquad 4.18$$

Thermal cycles in $< P >$ and $< L >$ are then observed from three points of view:

* Where the lattice spacing is set to 1 and e is absorbed into the fields

1) α fixed , varying β.

2) β fixed , varying α.

3) Varying both α and β.

Only a small number of Monte Carlo iterations (50 - 100) were used for each point due to the large computations involved at each link and site. Hence the occurrence of hysterisis loops in the thermal cycles is taken as the signal for phase transitions - see fig. 1. With this limited data, however, we cannot be sure of the order of the transitions.

Combining results for $< P >$ and $< L >$ from (1) and (2) we find evidence for three phases in the models $n = 2,3$. Using diagonal scans as in (3) we see clearly that the transition line C shows up in both $< P >$ and $< L >$. However, the spin ordering transition B shows up only in $< L >$ while the gauge transitions A is noticed only by $< P >$. This effect may be understood by considering the free energy density $\Gamma(\alpha,\beta) = \ln Z(\alpha,\beta)$ on either side of a given phase boundary. Assuming Γ to be analytic within each phase we have :

$$d\Gamma = \frac{\partial \Gamma}{\partial \alpha} d\alpha + \frac{\partial \Gamma}{\partial \beta} d\beta$$

$$= \frac{d-1}{2} < P > d\alpha + < L > d\beta \qquad 4.19$$

Suppose there exists a discontinuous jump in Γ between two phases I and II (as in a first-order transition) then we can write

$$d\Gamma_I = d\Gamma_{II} . \qquad 4.20$$

Then from (4.19)

$$\frac{d-1}{2}\left(\langle P\rangle_I - \langle P\rangle_{II}\right)d\alpha = \left(\langle L\rangle_{II} - \langle L\rangle_I\right)d\beta \qquad 4.21$$

ie.
$$\frac{d\alpha}{d\beta} = -\frac{2}{d-1}\,\frac{\Delta\langle L\rangle}{\Delta\langle P\rangle} \qquad 4.22$$

Thus the ratio of discontinuities in $\langle L\rangle$ and $\langle P\rangle$ is determined simply by the orientation of the phase boundary in the (α,β) plane. Note that since $\langle L\rangle$ and $\langle P\rangle$ are both positive the slope of the boundary must be negative.

For higher-order transitions corrections to (4.20) will appear. In this case (4.22) may be thought of as the ratio of leading singularities in $\langle P\rangle$ and $\langle L\rangle$. The strength of these singularities might then determine the relative extent to which the transitions show up in $\langle P\rangle$ and $\langle L\rangle$.

4. Mean field theory and masses.

In order to extract some of the physics in each phase we turn to the mean field approximation reviewed in Chapter two. We summarise the results here and some details are given in appendix C.

Elitzur's theorem.

Within the mean field approach it is natural to follow the example of the spin theory and determine self-consistently the average values of the fields $\langle U_x^\mu\rangle$ and $\langle Z_x^a\rangle$. For locally invariant theories however, this apparently contradicts Elitzur's theorem* which requires that both these quantities should vanish. Despite this, some results have been obtained in impressive agreement with Monte Carlo data [13]. Since the average fields are gauge dependent

* Referenced in Chapter three

quantities it might seem natural to fix a gauge as a way round this problem [14]. However, it has been shown [15] that at least for the axial gauge $<U_x^\mu>$ still vanishes rigorously.

For the coupled system considered here, a qualitatively identical phase diagram is obtained with or without gauge fixing [1]. In what follows we use an unfixed scheme to firstly obtain a phase diagram for comparison with the Monte Carlo results of section three. These results are in good agreement and we go on to compute various masses.

The phases

For the coupled system the self-consistency equation 2.20 on the sites of the spin model is replaced by a pair of self-consistency conditions on the site and link expectation values. In the case of symmetry breaking the Z^a are rotated and a gauge transformation is made so that both $<U^\mu> = <C>$ and $<Z^a> = <X>$ are real.

The corresponding mean fields are :

$$h_c = 2(d-1)\,\alpha <c>^3 + \beta <x>^2 + J_c \qquad 4.23$$

$$h_x = 2d\,\beta <c><x> + J_x$$

Expectation values are obtained using the 'partition functions':

$$Z_c(h_c) = \int D\theta \exp\{c \cdot h_c\}$$

$$Z_x(h_x) = \int D Z^a D\bar{Z}^a \delta(Z^a \bar{Z}^a - 1) \exp\{x \cdot h_x\} \qquad 4.24$$

and self-consistency gives the results for $<c>$ and $<x>$:

$$<c> = I_1(h_c) / I_0(h_c)$$

$$<x> = I_n(h_x) / I_{n-1}(h_x) \qquad 4.25$$

The phase boundaries are then determined in the same way as the spin model from the thermodynamic free energy $\Gamma(<c>,<x>)$:

$$\Gamma(<c>,<x>) = 2d\beta<c><x>^2 + \frac{3}{2} d(d-1)\alpha <c>^4 + J_x<s> + dJ_c<c>$$

$$- \ln Z_x(h_x) - d \ln Z_c(h_c) \qquad 4.26$$

The resulting phase diagram is compared with the Monte Carlo results in figs. 2 , 3 with $n = 2,3$.

We find (incorrectly) a first-order transition beginning at the pure $U(1)$ transition point and continuing through the triple point up to the CP^{n-1} axis at $\alpha = 0$. On the other hand the transition line from the $O(2n)$ axis at $\alpha = \infty$ leading to the triple point is second-order in this approximation. This result is not inconsistent with the expected behaviour of $O(4)$ and $O(6)$ spin models.

Masses*

In the mean field calculation for the coupled system we find a mixing occurs between site and link expectation values. As a result no simple formula for the σ mass analogous to (1.39) may be obtained for the Green's function in position space. Hence we consider the momentum space derivation of Chapter two. The mixing still occurs

* See Acknowledgements.

but was found to be manageable. The calculations are outlined in appendix C. The results are as follows:

a) 'Confining region' - small α, small β

In the symmetric phase (small β) $< Z^a > = 0$ for all a, and there are $2n$ degenerate scalar fields given by

$$m^2_{Z,\bar{Z}} = \frac{2n}{<c>\beta} - 2d \qquad 4.27$$

where $\beta \leq \beta_c = \frac{n}{d<c>}$ for the symmetric phases.

However, in this first region α is also small, we have $< c > = 0$ and so all the masses are infinite. Thus confinement occurs but for trivial reasons - in fact the same argument may be used to find bound states, eg. $< Z^a_x \bar{Z}^b_x >$ of infinite mass !

b) Maxwell phase - large α , small β

Here $c \neq 0$ and(4.27)gives a set of $2n$ degenerate massive scalars.

There are $2d$ modes of fluctuation in the link value $< U^\mu >$. Of these d are massless transverse modes (see proof C1). One of these is the unphysical gauge degree of freedom, while $d-1$ are the photon.

The remaining d modes are massive and remain so in the continuum limit $\beta \to \beta_c$ where $m^2_{Z,\bar{Z}} \to 0$.

c) Higgs phase

In the remaining region we have an example of the Higgs mechanism [16]. The photon is massive:

$$m_\gamma^2 = \frac{\beta}{\alpha}\frac{\langle \varkappa \rangle^2}{\langle C \rangle^3} > 0 \qquad 4.28$$

with d-1 polarizations.

There are now 2n-2 massless Goldstone bosons (See appendix C and Chapter one) and a massive scalar field σ. The calculation of m_σ^2 involves mixing between $\langle Z^a \rangle$ and the longitudinal mode in $\langle U^\mu \rangle$ (The physical σ is identified with the state having lower mass which tends to zero as $\beta \to \beta_c$), and is omitted here.

5. Discussion

As $n > 1$ more spins have been added than are necessary to break the gauge symmetry. The existence in these models of a phase boundary separating Higgs and confinement phases is in sharp contrast to the case $n = 1$ [5,7].

For $n = 1$ a similar effect is achieved however, when the Higgs field carries multiple (integer) charge q. The action then reads

$$S = \alpha \sum_{x,\mu\nu} \cos[aeF_{\mu\nu}] + \beta \sum_{x,\mu} \cos[\Delta_\mu \theta_x - qA_x^\mu] \qquad 4.29$$

In this case, when $q = 1$ it has been shown that the two phases are continuously connected [4].

As the model here has two coupling constants it is possible to demonstrate renormalization group flows within the phase diagram (see Chapter one). Bad statistics meant that Monte Carlo calculations of masses were unfeasible, but some results were obtained in the mean field approximation [17].

In order that the physics remains the same along contours in the phase diagram we require that the couplings α and β depend on on the lattice cutoff, Λ^2 say, in such a way that both m_γ^2 and m_σ^2 (in the Higgs phase) remain constant as Λ varies, i.e.

$$m_\gamma^2(\alpha,\beta) = f(\alpha,\beta)\Lambda^2$$

$$m_\alpha^2(\alpha,\beta) = g(\alpha,\beta)\Lambda^2 \qquad 4.30$$

Computing the ratio m_σ^2/m_γ^2 then eliminates the Λ^2 dependence of (4.30) and the mean field results for m_σ^2 and m_γ^2 give the contours of fig.4 .

The flows of constant mass ratio are in the direction of increasing m_σ^2 . The effect of a second-order transition is seen clearly near the Higgs/Maxwell boundary where $m_\sigma^2 \to 0$ rapidly. In this lowest order mean field approximation we would expect these lines to hit the boundary at some point. If the second-order transition were to persist in higher orders however, we would expect the flows to tend only asymptotically to the boundary.

However, a calculation in the corresponding continuum field theory [18] indicates a first-order transition (for $n \leq 365$) separating Higgs and Maxwell phases. If this result is true in the limit $\lambda \to \infty$ applying to the present model than we might expect the lattice mean field prediction of a second-order transition to be incorrect, except of course at the point $\alpha = \infty$ where it becomes the $O(2n)$ Heisenberg model.

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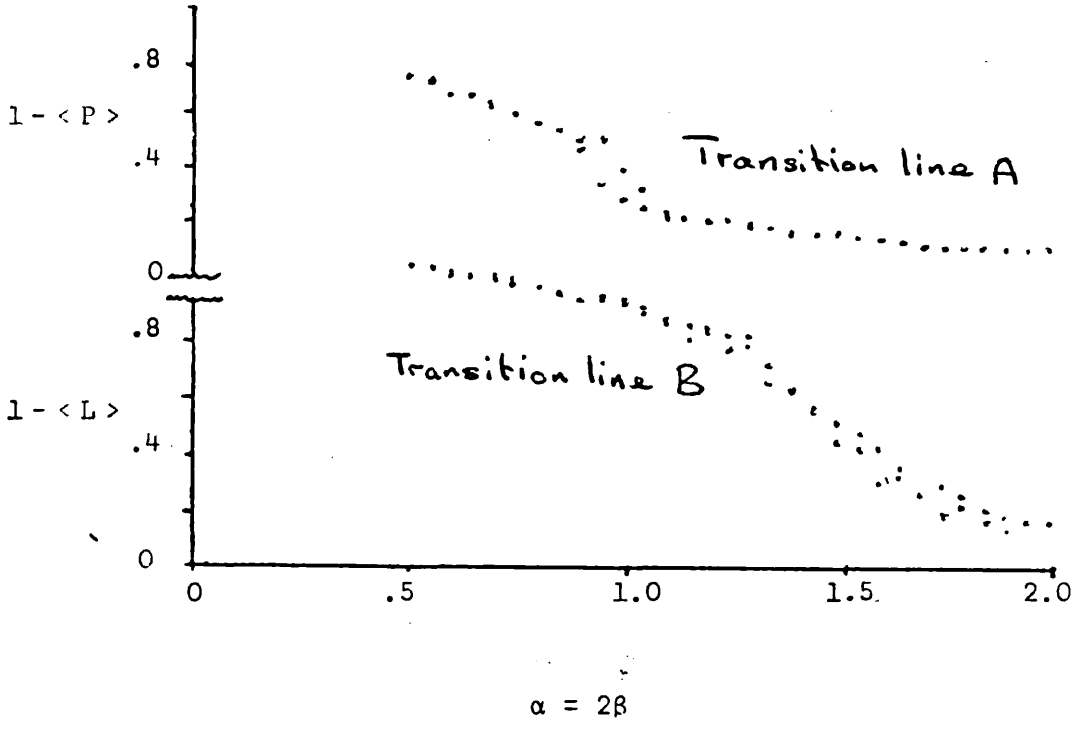


Fig. 1.

Diagonal scan for the line $\alpha = 2\beta$ when $n = 2$ (see fig. 2). Only 100 sweeps of the lattice were made for each point, averaging over the last 70.

Different transitions show up in $< L >$ and $< P >$.

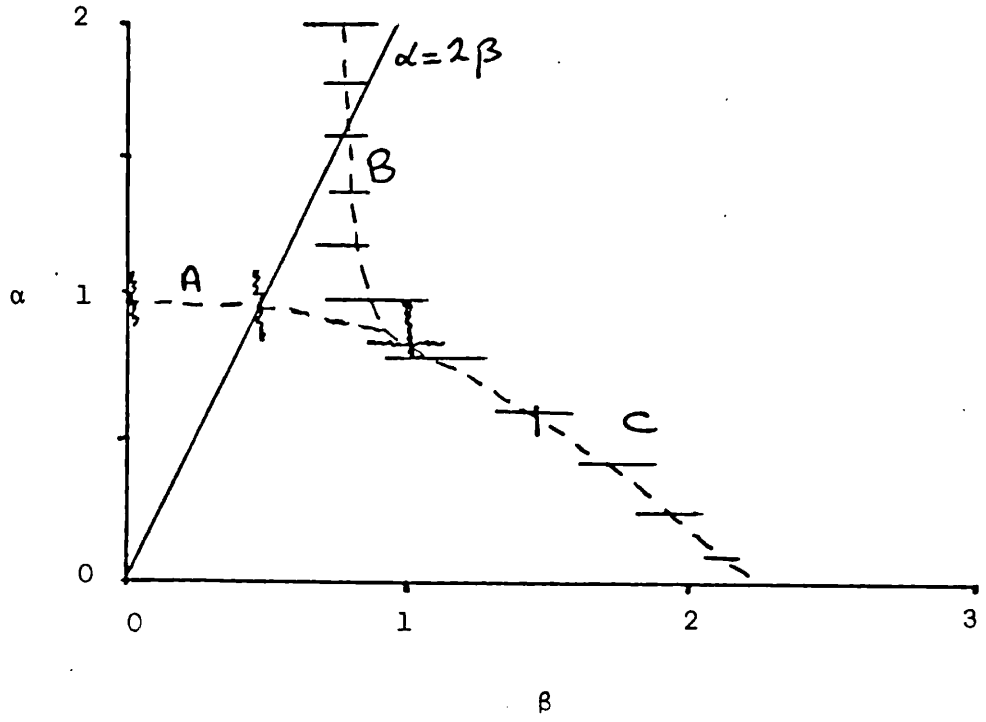


Fig. 2

Phase diagram for $n = 2$ on a 4^4 lattice obtained by Monte Carlo simulation. Horizontal and vertical bars indicate the approximate size of regions of slow convergence in $\langle L \rangle$ and $\langle P \rangle$ respectively. The line OAB indicates the path of the thermal cycle of fig. 1.

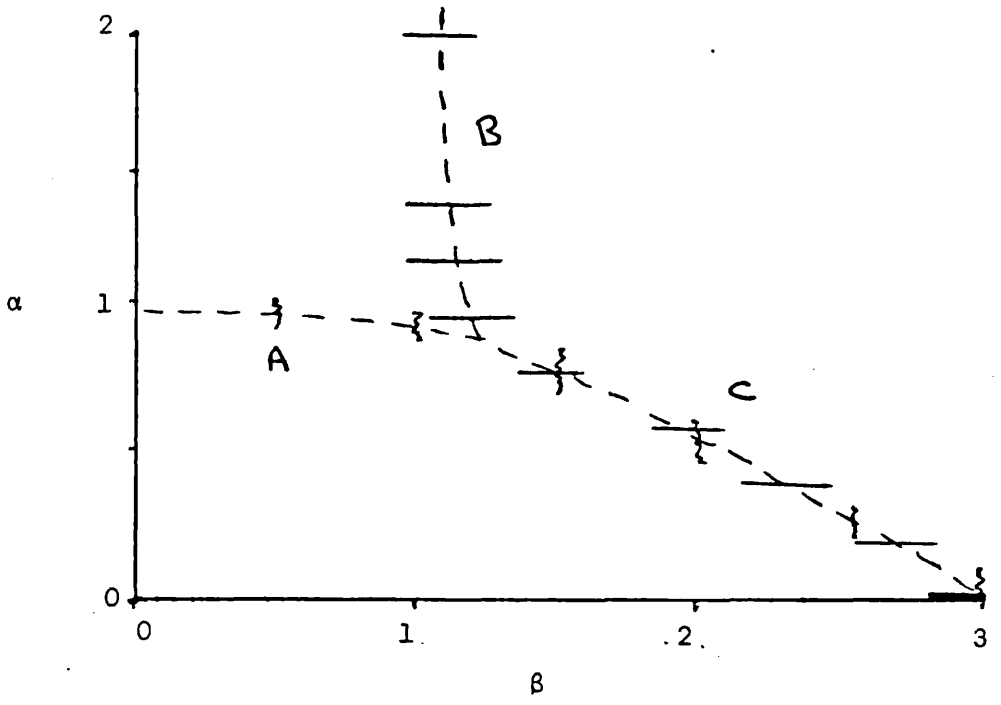


Fig. 3

As for fig. 2 but with $n = 3$.

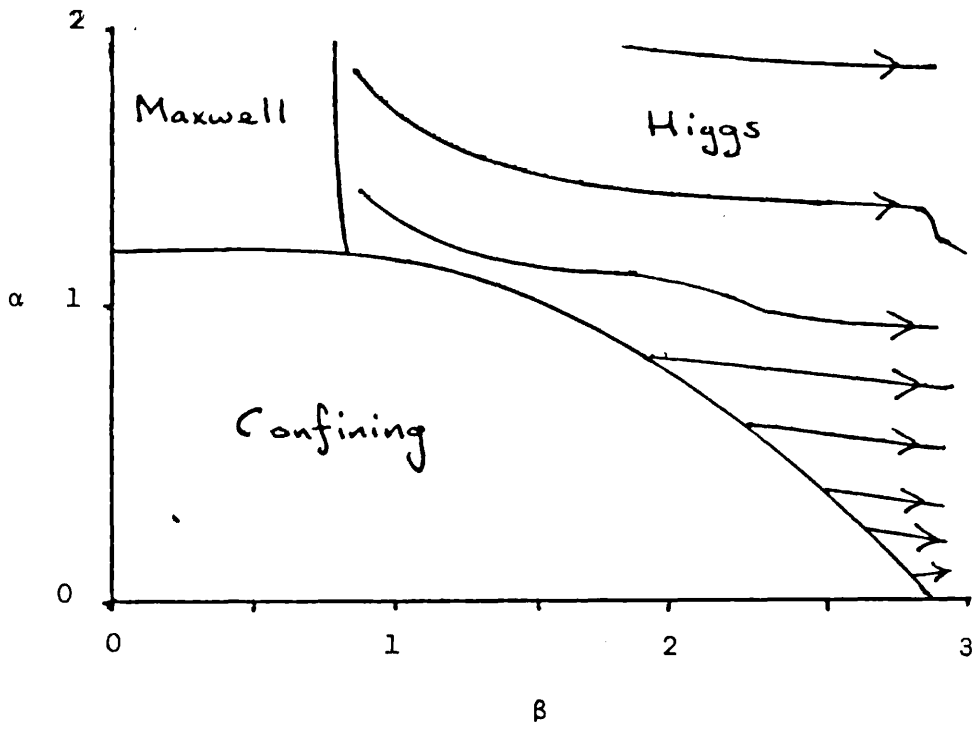


Fig. 4

Phase diagram for $n = 3$, obtained in the mean field approximation. The flow indicated in the Higgs phase is in the direction of increasing m_σ^2, keeping m_γ^2/m_σ^2 fixed.

APPENDIX A

I High temperature expansion (low β)

Since we are only concerned here with low order in β, diagrams are obtained directly from expanding the exponential in Z, rather than from the more powerful method of performing a character expansion first [1] :

$$Z(\beta) = \int \prod_x D\phi_x \delta(\phi_x^2 - 1) \exp\{\beta \sum_{x,\mu} \phi_{x+\mu} \cdot \phi_x\}$$

$$\sim \int \prod_x D\phi_x \, \delta(\phi_x^2 - 1) \prod_{x,\mu} [1 + \beta \phi_{x+\mu} \cdot \phi_x + \frac{1}{2!} \beta^2 (\phi_{x+\mu} \cdot \phi_x)^2 + \ldots] \quad \text{A1.1}$$

Any term in the product $\prod_{x,\mu}$ that is not invariant to the measure on all sites within the term will vanish. The remaining terms depend numerically on n and the size and dimension of the lattice, and can be represented as a sum of diagrams.

Clearly, only even powers of ϕ_x are invariant to the measure $D\phi_x \, \delta(\phi_x^2 - 1)$ so we write

$$Z(\beta) = \sum_{k=0}^{\infty} \beta^{2k} \tilde{Z}_{2k} \quad \text{A1.2}$$

To evaluate $\tilde{Z}_{2k}$ consider the following results. Let ϕ_x^i, $i = 1, 2, \ldots, n$ be the vector components at a given site x and define

$$\langle \phi^i \phi^j \rangle_x := \int D\phi_x \, \delta(\phi_x^2 - 1) \, \phi_x^i \phi_x^j \quad \text{A1.3}$$

Then clearly

$$\langle \phi^i \phi^j \rangle_x = A \delta_{ij} \quad \text{A1.4}$$

The normalization condition $1 = \langle 1 \rangle$ implies

$$1 = \langle 1 \rangle = \langle \phi^2 \rangle = An \quad , \quad \text{so}$$

$$\langle \phi^i \phi^j \rangle_x = \frac{\delta_{ij}}{n} \qquad \text{A1.5}$$

Higher order expressions may be obtained by combining indices in all possible ways:

$$\langle \phi^i \phi^j \phi^k \phi^\ell \rangle_x = B(\delta_{ij}\,\delta_{k\ell} + \delta_{ik}\,\delta_{j\ell} + \delta_{i\ell}\,\delta_{jk}) \qquad \text{A1.6}$$

Contracting over k and ℓ implies

$$\frac{1}{n}\,\delta_{ij} = \langle \phi^i \phi^j \phi^2 \rangle_x = B(n+2)\,\delta_{ij} \quad , \quad \text{so}$$

$$B = \frac{1}{n(n+2)} \quad .$$

Diagrams for $\tilde{Z}_{2k}$ may now be evaluated by combinations of the single site integrals A1.5, A1.6.

$\tilde{Z}_0$

$$\tilde{Z}_0 = 1 \quad , \qquad \text{the trivial order} \qquad \text{A1.7}$$

$\tilde{Z}_2$

$$\tilde{Z}_2 = \frac{1}{2!}\,C_1 \langle \phi^i \phi^j \rangle_x \langle \phi^i \phi^j \rangle_{x+\mu}$$

$$= \frac{1}{2!}\,C_1\,\delta_{ij}\delta_{ij}/n^2$$

$$= \frac{1}{2!}\,C_1/n \quad . \qquad \text{A1.8}$$

C_1 is the factor associated with the possible positions of the diagram on the lattice. In this case a single link oriented twice:

Hence $C_1 = d\,N^d$, the number of links on a finite lattice and

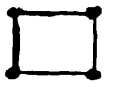
$$\mathcal{Z}_2 = \frac{dN^d}{2n} \qquad \text{A1.9}$$

$\mathcal{Z}_4$

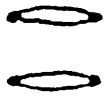
There are four different diagrams:

$$\text{(i)} \qquad = C_2 \langle \phi^i \phi^j \rangle_x \langle \phi^j \phi^k \rangle_{x+\mu} \langle \phi^k \phi^\ell \rangle_{x+\mu+\nu} \langle \phi^\ell \phi^i \rangle_{x+\nu} \qquad \text{A1.10}$$

Each bracket contributes a factor $\frac{1}{n}$ from the integration, while contracting over the indices gives a factor n. $C_2 = \frac{1}{2} dN^d(d-1)$, the number of plaquettes on a lattice. Hence A1.9



$$= \frac{1}{2} dN^d(d-1)/n^3 \qquad \text{A1.11}$$



$$\text{(ii)} \qquad = C_3 [\tfrac{1}{2!} \langle \phi^i \phi^j \rangle_x \langle \phi^i \phi^j \rangle_{x+\mu}]^2 \qquad \text{A1.12}$$

$$= C_3/4n^2$$

$$= \frac{1}{2} dN^d(dN^d - (4d-1))/4n^2 \qquad \text{A1.13}$$

$$\text{(iii)} \qquad = \frac{1}{2!2!} \langle \phi^i \phi^j \rangle_x \langle \phi^i \phi^j \phi^k \phi^\ell \rangle_{x+\mu} \langle \phi^k \phi^\ell \rangle_{x+\mu+\nu} \qquad \text{A1.14}$$

$$= C_4 \frac{1}{2!2!} \times \frac{1}{n} \times \frac{1}{n(n+2)} \times \frac{1}{n} \times n(n+2)$$

where the last factor arises from contractions over the deltas.

$$= C_4/4n^2$$

$$= dN^d(2d-1)/4n^2 \qquad \text{A1.15}$$

$$\text{(iv)} \qquad = C_5 \frac{1}{4!} \langle \phi^i \phi^j \phi^k \phi^\ell \rangle_x \langle \phi^i \phi^j \phi^k \phi^\ell \rangle_{x+\mu} \qquad \text{A1.16}$$

$$= C_5 \frac{1}{4!} \times \frac{1}{n^2(n+2)^2} \times (\delta_{ij}\delta_{k\ell} + \ldots, + \delta_{i\ell}\delta_{jk})^2$$

The last factor gives 9 terms and turns out to be $3n(n+2)$, so

$$= C_5 \; / \; 8n(n+2)$$

$$= dN^d \; / \; 8n(n+2) \qquad \text{A1.17}$$

Summing the diagrams we have an expression for $Z(\beta)$ to order β^4 :

$$Z(\beta) \simeq 1 + \frac{dN^d}{2n}\beta^2 + dN^d\left[\frac{1}{8n(n+2)} + \frac{2d-1}{4n^2} + \frac{d-1}{2n^3} + \frac{dN^d - 4d+1}{8n^2}\right]\beta^4 + O(\beta^6)\ldots \qquad \text{A1.18}$$

$F(\beta) = \ln Z(\beta)$ is the free energy and differentiating F with respect to β gives the average energy density $E(\beta)$ of 2.5 to $O(\beta^3)$:

$$E(\beta) = \beta/n + \left(\frac{2d}{n^2} - \frac{3n+4}{n^2(n+2)}\right)\beta^3 + O(\beta^3) + \ldots$$

As an informative check we calculate E directly from diagrams :

$$E(\beta) = Z^{-1}(\beta)\,\frac{1}{dN^d}\sum_{x,\mu}\int \prod_x D\phi_x\,\delta(\phi_x^2 - 1)\;\phi_{x+\hat\mu}\,\phi_x\,\exp\{\beta\sum_{x,\mu}\phi_{x+\hat\mu}\,\phi_x\} \qquad \text{A1.20}$$

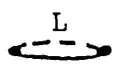
A1.20 is evaluated at a fixed link $\phi_{a+\hat\mu}\,\phi_a = L$ somewhere on the lattice - since the system is translationally invariant, any one link will do.

A diagram will now be non-zero where every site on the diagram belongs to either:

a) an even power of links from the $\prod_{x,\mu}$ in the expansion of A1.17.

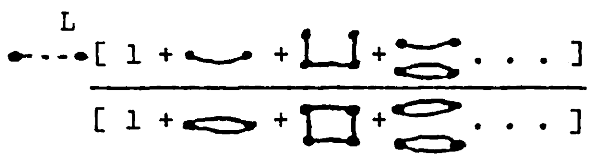
b) an odd power of links from the $\prod_{x,\mu}$ and to L .

Hence the lowest order diagram is simply

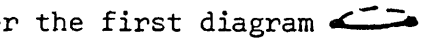


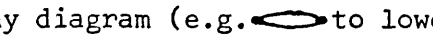
$= \beta/n$ A1.21

Each such diagram can occur with all possible sets of disconnected diagrams from $Z(\beta)$, i.e.

$E(\beta) =$  A1.22

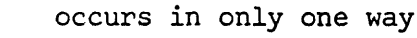
When all diagrams are considered the two bracketed series do not quite cancel, since the top bracket is a sum over all diagrams in $Z(\beta)$ on the lattice except for those including L.

i) Consider the first diagram  giving a factor β/n .

Now any diagram (e.g.  to lowest order) from $\Pi^{x,\mu}$ in the expansion of A1.17 with sites in common with must be subtracted. To this low order there are two kinds:

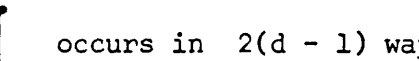
1) occurs $(4d - 2)$ ways so using previous considerations we subtract

$$\frac{1}{2}(4d - 2)\beta^3/n^2 \qquad \text{A1.23}$$

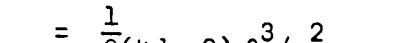
2)  occurs in only one way, hence subtract

$$\frac{1}{2}\beta^3/n^2 \qquad \text{A1.24}$$

With $O(\beta^3)$ corrections taken care of, we evaluate the positive β^3 contributions in a similar fashion to $Z(\beta)$:

(ii)  occurs in $2(d - 1)$ ways for given link L, therefore it gives

$$2(d-1)\beta^3/n^3 \qquad \text{A1.25}$$

(iii)  $= \frac{1}{2}(4d - 2)\beta^3/n^2$ A1.26

(which cancels exactly with (1))

(iv) $= \beta^3/2n(n+2)$ A1.27

The next terms and corrections are $O(\beta^5)$. To order β^3 we have

$$E(\beta) = \beta/n + \left(\frac{2d}{n^2} - \frac{3n+4}{n^2(n+2)}\right)\beta^3 \ . \ . \ . \quad \text{as before} \qquad \text{A1.28}$$

II Low temperature expansion (high β)

The general method is the standard perturbation expansion for the Green's functions in field theory, based around Z_o, the free field generating functional. The case of an $O(n)$ symmetric Lagrangian is given in ref. [2].

The following basic results are easily derived from the momentum space transformation

$$\phi_x \to \sum_{q=-\pi}^{+\pi} e^{iq.x} \tilde{\phi}_q$$

where

$$\tilde{\phi}_p := N^{-d} \sum_x e^{-ip.x} \phi_x$$

using $$\sum_x e^{i(p-q)\cdot x} = N^d \sum_{n=-\infty}^{+\infty} \delta_{p,\, q+2n\pi}$$

1) $$\sum_x \phi_x^1 \phi_x^2 \ldots \phi_x^k = N^d \sum_{p_1,p_2,\ldots,p_{k-1}} \tilde{\phi}^1_{p_1} \tilde{\phi}^2_{p_2} \ldots \tilde{\phi}^{k-1}_{p_{k-1}} \tilde{\phi}^k_{-p_1,-p_2,\ldots,-p_{k-1}} \qquad \text{A2.1}$$

where momentum is understood to be conserved only modulo 2π

2) By translational invariance and using A2.1

$$\sum_{x,\mu} (\phi_{x+\mu} - \phi_x)^2 = \sum_{x,\mu} (2\phi_x^2 - 2\phi_{x+\mu}\phi_x)$$

$$= N^d \tilde{\phi}_p \tilde{\phi}_{-p} \Delta_p^{-1} \qquad \text{A2.2}$$

where $$\Delta_p^{-1} := \sum_\mu (2 - 2\cos p_\mu) \ .$$

The partition function 2.2 for the Hamiltonian in the absence of external fields reads :

$$Z(\beta) = \int \prod_x D\phi_x \delta(\phi_x^2 - 1) \exp\{\beta \sum_{x,\mu} [1 - \tfrac{1}{2}(\phi_{x+\mu} - \phi_x)^2] \}$$

writing the fields $\phi_x = (\sigma_x, \pi_x)$ σ_x scalar, $\pi_x = (\pi_x^1, \pi_x^2, \ldots, \pi_x^{n-1})$

$$\alpha \int \prod_x D\pi_x D\sigma_x \delta(\sigma_x^2 - [1 - \pi_x^2]) \exp\{-\frac{\beta}{2} \sum_{x,\mu} [(\sigma_{x+\mu} - \sigma_x)^2 + (\pi_{x+\mu} - \pi_x)^2] \} \qquad \text{A2.3}$$

The fixed length condition gives interactions by :

$$d\phi_x \delta(\phi_x^2 - 1) = d\pi_x \, d\sigma_x \, \delta(\sigma_x^2 - [1 - \pi_x^2])$$

$$= \tfrac{1}{2} d\pi_x (1 - \pi_x^2)^{-\frac{1}{2}}$$

$$= \tfrac{1}{2} d\pi_x \exp\{-\tfrac{1}{2} \ln(1 - \pi_x^2)\}$$

Transforming to momentum space A2.3 reads

$$Z(\beta) \alpha \int \prod_p d\pi_p \exp\{H_F + H_I\} \qquad \text{A2.4}$$

where $H_F = -\frac{N^d \beta}{2} \sum_p \pi_p \cdot \pi_{-p} \Delta_p^{-1}$

$$H_I = -\frac{N^d \beta}{2} \sum_p \sigma_p \sigma_{-p} \Delta_p^{-1} - \frac{N^d}{2} \sum_p \ln(1 - \pi_p \cdot \pi_{-p}) .$$

At low temperature, spins tend to align in the σ direction, say. Oscillations around σ are assumed to be small, hence $|\pi_x| << 1$ and we write :

$$\sigma_x = (1 - \pi_x)^{\frac{1}{2}} \simeq 1 - \tfrac{1}{2}\pi_x^2 - \tfrac{1}{8}\pi_x^4 \ldots$$

and $$\ln(1 - \pi_x^2) \simeq -\pi_x^2 - \tfrac{1}{2}\pi_x^4 \ldots .$$

Up to quartic terms, H_I then is

$$H_I \simeq -\frac{N^d\beta}{8} \sum_{p_1,p_2,p_3} (\pi_{p_1}\cdot\pi_{p_2})\Delta^{-1}_{p_1+p_2}(\pi_{p_3}\cdot\pi_{-p_1-p_2-p_3}) + \ldots$$

$$+ \frac{N^d}{2}\sum_p \pi_p\cdot\pi_{-p} + \frac{N^d}{4}\sum_{p_1,p_2,p_3}(\pi_{p_1}\cdot\pi_{p_2})(\pi_{p_3}\cdot\pi_{-p_1-p_2-p_3}) + \ldots \quad \text{A2.5}$$

Adding source terms $J_p.\pi_{-p}$ for the π_p fields and making the usual replacement $\pi_p \to \frac{\delta}{\delta J_{-p}}$ we pull $\exp\{H_I(\frac{\delta}{\delta J_{-p}})\}$ outside the integral A2.4, leaving the Caussian form with the π_p integration range extended to $\pm\infty$:

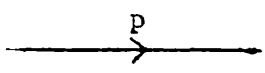
$$Z_F(\beta) = \int_{-\infty}^{+\infty}\prod_p D\pi_p \exp\{-\frac{N^d\beta}{2}\sum_p \pi_p\cdot\pi_{-p}\,\Delta_p^{-1} + N^d\sum_p J_p.\pi_{-p}\}$$

$$\alpha \exp\{\frac{N^d}{2\beta}\sum_{p\neq 0} J_p.J_{-p}\,\Delta_p\} \quad \text{A2.6}$$

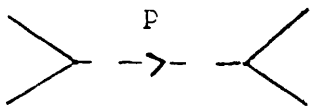
Note that the $p=0$ mode is excluded in order that the 'propagator' Δ_p be well defined. The integral over the $p=0$ mode of ϕ_p may be taken out right at the beginning since it contributes a numerical factor which cancels with Z in the denominator for averages over $O(n)$ invariant quantities.

A set of 'Feynman rules' may be given in the normal way. Note that diagrams for the $O(n)$ theory will contain factors δ_{ij} $i, j = 1, \ldots, n-1$ leading to a factor $n-1$ for all closed π_p loops.

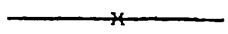
Diagrams



$$\leftrightarrow \quad \frac{N^{-d}}{\beta}\Delta_p \quad \text{A2.7}$$



$$\leftrightarrow \quad -N^d\beta\,\Delta_p^{-1} \quad \text{A2.8}$$



$$\leftrightarrow \quad N^d \text{ from the measure.} \quad \text{A2.9}$$

In addition to closed index loops, any closed loop will involve a sum $\sum_p$ over all p for which every propagator in the loop has non-zero momentum.

Evaluation of $E(\beta)$

$$E(\beta) = \langle N^{-d}\, d^{-1} \sum_{x,\mu} \phi_{x+\mu}\phi_x \rangle = N^{-d}\, d^{-1} \langle \sum_{x,\mu} [1 - \tfrac{1}{2}(\phi_{x+\mu} - \phi_x)^2] \rangle$$

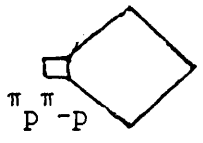
$$= 1 - d^{-1} \langle \sum_p \tfrac{1}{2}\, \phi_p \cdot \phi_{-p}\ \Delta_p^{-1} \rangle$$

$$\sim 1 - \frac{1}{2d} \langle \sum_p \pi_p \cdot \pi_{-p}\ \Delta_p^{-1} \rangle - \frac{1}{8d} \langle \sum_{p_1,p_2,p_3} (\pi_{p_1} \cdot \pi_{p_2}) \Delta_{p_1+p_2}^{-1} (\pi_{p_3} \cdot \pi_{-p_1-p_2-p_3}) \rangle$$

A2.10

(i) The first bracket of 2.7 gives :

(a) $\pi_p \cdot \pi_{-p}$ acting on the free part of Z, i.e. the 'tree level' diagram



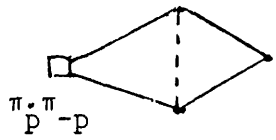
$$= (n-1)\, \frac{N^{-d}}{\beta} \sum_{p \neq 0} \Delta_p^{-1}\, \Delta_p$$

$$= (n-1)\, \frac{N^{-d}}{\beta}\, (N^d - 1) \qquad \text{A2.11}$$

The N^d dependence is apparent even at this lowest order. For $N^d \to \infty$ we have

$$E(\beta) \sim 1 - \frac{(n-1)}{2d\,\beta} + O(\beta^{-2}) \ldots \qquad \text{A2.12}$$

b) $\pi_p \cdot \pi_{-p}$ combined with interaction terms from Z, giving contributions $O(\beta^{-2})$. Expressions arise :



$$= -\frac{(n-1)}{\beta^2} N^{-2d} \sum_{p_1,p_2} \Delta_{p_2} \Delta^{-1}_{p_1+p_2} \Delta_{p_2}$$

The non-trivial sum may be evaluated in the large N limit, or summed directly on a computer.

(ii) The second bracket of A2.10 also gives $O(\beta^{-2})$ terms from acting are the free part of Z.

The final N dependent result for $E(\beta)$ is

$$E(\beta) \simeq 1 - \frac{(n-1)}{2d\beta} N^{-d}(N^d - 1) + \frac{(n-1)}{4d\beta^2} I \qquad \text{A2.13}$$

$$I = N^{-d} \sum_{p_1} \Delta_{p_1} [N^{-d} \sum_{p_2} \Delta^{-1}_{p_1+p_2} \Delta_{p_2} - 2]$$

In the large N limit I becomes $-\frac{1}{2d}$ and A2.13 is

$$E(\beta) \simeq 1 - \frac{n-1}{2d\beta} - \frac{n-1}{8d^2\beta^2} + O(\beta^{-3}) \ldots \qquad \text{A2.14}$$

References

[1] R. Balian, J.M. Drouffe and C. Itzikson, Phys. Rev. D11 (1975) 2104.

[2] D. Amit, Field Theory, the Renormalization Group and Critical Phenomena (McGraw Hill, London, 1978).

APPENDIX B

I High temperature (low α) expansion for U(1)

Expansions to very high order (up to α^{14}) have been carried out [1, 2] using character expansions. As an aid to the mixed model we simply list here the low order diagrams obtained from expanding the exponential in Z of (3.5) (putting a = 1)

$$Z(\alpha) = \int \prod_{x,\mu} D\theta^{\mu}_{x} \exp\{\alpha \sum_{x,\mu} \cos\theta_{\square}\}$$

$$\simeq \int \prod_{\ell} D\theta_{\ell} \prod_{\square} (1 + \alpha \cos\theta_{\square} + \frac{\alpha^2}{2!} \cos^2\theta_{\square} + \ldots) \qquad \text{B1.1}$$

where $\theta_{\ell} = \theta^{\mu}_{x}$ and $\theta_{\square} = \theta^{\mu}_{x} + \theta^{\nu}_{x+\mu} - \theta^{\mu}_{x+\mu+\nu} - \theta^{\nu}_{x+\nu}$

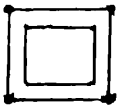
Using the results:

$$\int_0^{2\pi} d\theta \cos\theta = 0$$

and $$\frac{1}{2\pi} \int_0^{2\pi} d\theta_A \cos^2(\theta_A + \theta_B) = \frac{1}{2}$$

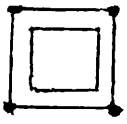
we see that in analogy with the spin models, only terms with an even number of links belonging to each plaquette in a given diagram will survive. Expanding Z as a set of diagrams we have:

$O(\alpha^2)$

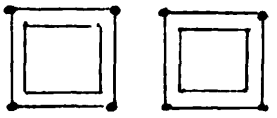


$= \frac{\alpha^2}{2!} N_{\square} \times \frac{1}{2}$ from integration B1.2

$O(\alpha^4)$

(i) 

$= \frac{\alpha^4}{4!} N_{\square} \times \frac{3}{8}$ B1.3

(ii)  $= \frac{\alpha^4}{2!2!} \ \frac{1}{2} N_{\square} (N_{\square} - [8d-1]) \times \frac{1}{4}$ (B1.4)

(iii)  $= \frac{\alpha^4}{2!2!} \times N_{\square} (4d-6) \times \frac{1}{4}$ (B1.5)

Calculations similar to those for the spin model yield the result (3.7) for $E(\alpha)$:

$$\langle E(\alpha) \rangle \ \underset{\sim}{\sim} \frac{\alpha}{2} - \frac{\alpha^3}{16} + \frac{1}{16} (d - \frac{11}{6}) \ \alpha^5 + O(\alpha^7) \ldots \qquad \text{(B1.6)}$$

II Low temperature (high α) expansion for U(1)

The method is again the general one of perturbation theory. A discussion of lattice weak coupling is given in [3].

As in continuum theory the calculation is only possible if a 'gauge' is chosen. When distances are large compared to the lattice spacing, i.e. for small momentum p. the results of continuum Q.E.D are recovered.

For large α we approximate (3.3):

$$S_{U(1)} \sim \sum_{x,\mu\nu} [1 - \frac{\theta^2_{x,\mu\nu}}{2!} + \frac{\theta^4_{x,\mu\nu}}{4!} + \ldots] \qquad \text{(B2.1)}$$

where $\theta_{x,\mu\nu} := (\Delta_\mu \theta^\nu_x - \Delta_\nu \theta^\mu_x)$

and $\Delta_\mu \theta^\nu_x = \theta^\nu_{x+\mu} - \theta^\nu_x$ is the lattice 'difference' operator with spacing a set to unity.

The generating functional Z_o is obtained as in the spin model from the quadratic part of (B2.1). Transforming $\theta^2_{x,\mu\nu}$ into momentum space yields the inverse propagator

$$M^{-1}_{\mu\nu} = 2N^d \left[\sum_\alpha (2 - 2\cos p_\alpha)\, \delta_{\mu\nu} + (\cos p_\mu + \cos p_\nu - \cos(p_\mu - p_\nu) - 1)\right] \qquad \text{B2.2}$$

This matrix is not invertible without the addition of a gauge fixing term, for instance

$$-\frac{1}{A}(\Delta_\mu\, \theta^\mu_x)^2$$

to the action (B2.1).

For suitable A we have the lattice 'Feynman gauge' and (B2.2) becomes

$$M^{-1}_{\mu\nu} = 2N^d \left[\sum_\alpha (2 - 2\cos p_\alpha)\right] \delta_{\mu\nu} \qquad \text{B2.3}$$

giving

$$M_{\mu\nu} = \frac{1}{2} N^{-d} \left[\sum_\alpha (2 - 2\cos p_\alpha)\right]^{-1} \delta_{\mu\nu} \qquad \text{B2.4}$$

For small p we recognize $M_{\mu\nu}$ as the ordinary massless propagator

$$M_{\mu\nu} \sim \frac{1}{p^2}\, \delta_{\mu\nu} \qquad \text{for small } p. \qquad \text{B2.5}$$

If required, a set of 'Feynman rules' could be written down in a similar fashion to the spin model.

III The heat bath algorithm in U(1) and SU(3)

Given a supply of uniformly distributed random numbers from a computer we need a way of transforming them into group elements U distributed with the Boltzmann weighting $P(U)\, dU$ of (1.51).

Suppose we write

$$P(U)\, dU = Q(U)\, d[R(U)] \qquad \text{B3.1}$$

where we require $0 < R < 1$.

Two cases arise:

(i) Q = constant.

If Q is independent of U we see immediately U may be generated according to (B3.1) by taking numbers $\hat{R}$ uniformly distributed on (0,1) and inverting $R(U)$.

(ii) $Q \neq$ constant.

In general the form of $P(U) \sim \exp\{\mathrm{Tr}\ \mathrm{Re}\, A^{\dagger} U\}$ is too complicated to allow us to define $R(U)$ in such a way as to make Q constant. However, we can still satisfy (B3.1) by firstly generating R uniformly and then correcting for the weight factor $Q(U)$.

Given a U generated as in (i), this defines a value of $Q = \hat{Q}$. Suppose we generate a new random number $\hat{R}'$ distributed uniformly on the range of $Q(U)$. Then if $\hat{R}' < \hat{Q}$ we reject $\hat{Q}$ and generate a new $\hat{R}$ and hence a new $\hat{Q}$. Thus the generated U that we finally accept is conditional on $\hat{Q}$ being accepted, i.e. the 'flat' distribution $d[R(u)]$ is multiplied by a factor $\int_0^Q dR'$ and so we have

$$\int_0^Q dR'\ d[R(u)] = Q(u)d[R(u)]\ . \qquad \text{B3.2}$$

The U(1) case

We are required here to generate θ according to:

$$P(\theta)\, d\theta = e^{M\cos\theta}\, d\theta \qquad 0 \leq \theta < \pi^{*} \qquad \text{B3.3}$$

* We need only solve (B3.3) for the half plane and then change $\theta \to -\theta$ with probability $\frac{1}{2}$.

Let

$$R(x) = (e^{Mx} - e^{-M})/(e^{M} - e^{-M}) \qquad \text{B3.4}$$

and $Q(x) = \exp\{M[\cos \pi/2\,(1-x) - x]\}$

where $x = 1 - 2\theta/\pi$

Then clearly (B3.3) becomes

$$P(\theta)\,d\theta \;\alpha\; Q(x)\,d[R(x)] \qquad \text{B3.5}$$

with $0 < R(x) \leq 1$.

Then selecting $\hat{R}$ uniformly on (0,1] gives x from the inverse function to R(x):

$$x = \frac{1}{M} \ln\{1 + (e^{2M} - 1)\,\hat{R}\} - 1 \qquad \text{B3.6}$$

To allow for the weighting Q(x) we take a second random number $\hat{R}$ and keep x if and only if:

$$\frac{Q(x)}{QMAX} > \hat{R}' \qquad \text{B3.7}$$

where Q_{MAX} is the maximum value of $Q(x) = e^{0.2105137\alpha}$ in this case.

The SU(3) case

The case of SU(3) is of course considerably more complicated. In the heat bath algorithm for SU(2) [4] one is able to make use of the fact that any sum of SU(2) matrices is proportional to another SU(2) element - thus the sum over surrounding plaquettes in the exponent of (1.59) is a single SU(2) matrix (times a factor).

For SU(3) however, this trick is out. The expression (B3.1) is decomposed into a weight factor Q(U), together with several factors $d[R_i(U)]$. Some details are given in ref. [5].

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APPENDIX C

Mean field calculation

Changing notation we recall the action (4.1):

$$S = \frac{\alpha}{2} \sum_{\square} [U^1U^2U^3U^4 + c.c.] + \frac{\beta}{2} \sum_{Z^a \; x\text{—}x \; \bar{Z}^{a'}} [Z^a U \bar{Z}^{a'} + c.c.] \qquad C1.1$$

and write $U^\ell = e^{i\theta^\ell} = c^\ell + i s^\ell \quad \ell = 1,\ldots,4$

$$Z^a = x^a + i y^a \qquad a = 1,\ldots,n$$

$$x^a x^a + y^a y^a = 1 \; .$$

Rewriting (C1.1) in terms of real and imaginary parts we have:

$$S = \alpha \sum_{\square} [c^1c^2c^3c^4 + s^1s^2s^3s^4 + (-s^1s^2c^3c^4 + s^1s^3c^2c^4 + s^1s^4c^2c^3 + s^2s^3c^1c^4 + s^2s^4c^1c^3 - s^3s^4c^1c^2)]$$

$$+ \beta \sum_{x\text{—}x \; Z^a \; \bar{Z}^{a'}} [x^a x^{a'} c + y^a y^{a'} c + y^a x^{a'} s - x^a y^{a'} s] \qquad C1.2$$

Given a site or link, (denoted x or in the following equations) mean values are associated with all the surrounding fields. Then the following expressions for the mean fields h are constructed from the relevant terms in (C1.2).

$$h_c = \alpha \sum_{\square} \langle c^2\rangle\langle c^3\rangle\langle c^4\rangle + \alpha \sum_{\square\square} [-\langle c^2\rangle\langle s^3\rangle\langle s^4\rangle + \langle c^3\rangle\langle s^2\rangle\langle s^4\rangle$$

$$+ \langle c^4\rangle\langle s^2\rangle\langle s^3\rangle + \langle c^5\rangle\langle s^6\rangle\langle s^7\rangle + \langle c^6\rangle\langle s^5\rangle\langle s^7\rangle - \langle c^7\rangle\langle s^5\rangle\langle s^6\rangle]$$

$$+ \beta[\langle x^a\rangle\langle x^{a'}\rangle + \langle y^a\rangle\langle y^{a'}\rangle] + J_c \qquad C1.3a$$

$$h_s = \alpha \sum_{\substack{3 \\ 4 \square 2}} \langle s^2\rangle\langle s^3\rangle\langle s^4\rangle + \sum_{\substack{3 \\ 4 \square 2 \\ 7 \square 5 \\ 6}} [-\langle s^2\rangle c^3\rangle\langle c^4\rangle + \langle s^3\rangle\langle c^2\rangle\langle c^4\rangle$$

$$+ \langle s^4\rangle\langle c^2\rangle\langle c^3\rangle + \langle s^5\rangle\langle c^6\rangle\langle c^7\rangle + \langle s^6\rangle\langle c^5\rangle\langle c^7\rangle - \langle s^7\rangle\langle c^5\rangle\langle c^6\rangle]$$

$$+ \beta[\langle y^a\rangle\langle x^{a'}\rangle - \langle x^a\rangle\langle y^{a'}\rangle] + J_s \qquad \text{Cl.3b}$$

$$h_x^a = \beta \sum_{\longrightarrow\!\!\!\!\!\!\times} \langle c\rangle\langle x^{a'}\rangle + \beta\{ \sum_{\times\!\!\!\!\!\!\longleftarrow} \langle s\rangle\langle y^{a'}\rangle - \sum_{\longrightarrow\!\!\!\!\!\!\times} \langle s\rangle\langle y^a\rangle\} + J_x^a \qquad \text{Cl.3c}$$

$$h_y^a = \beta \sum_{\longrightarrow\!\!\!\!\!\!\times} \langle c\rangle\langle y^{a'}\rangle + \beta\{ \sum_{\longrightarrow\!\!\!\!\!\!\times} \langle s\rangle\langle x^{a'}\rangle - \sum_{\times\!\!\!\!\!\!\longleftarrow} \langle s\rangle\langle x^a\rangle\} + J_y^a \qquad \text{Cl.3d}$$

Then the self-consistency conditions are:

$$\langle c\rangle = Z_1^{-1} \int D\,\theta\, C \exp\{ ch_c + sh_s \} \qquad \text{Cl.4a}$$

$$\langle s\rangle = Z_1^{-1} \int D\,\theta\, S \exp\{ ch_c + sh_s \} \qquad \text{Cl.4b}$$

$$\langle x^a\rangle = Z_2^{-1} \int DX\,DY\, x^a \exp\{x^a h_x^a + y^a h_y^a\} \qquad \text{Cl.4c}$$

$$\langle y^a\rangle = Z_2^{-1} \int DX\,DY\, y^a \exp\{x^a h_x^a + y^a h_y^a\} \qquad \text{Cl.4d}$$

where $Z_1 = \int D\theta \exp\{ch_c + sh_s\}$

$Z_2 = \int DX\,DY \exp\{x^a h_x^a + y^a h_y^a\}$ Cl.5

and the site measure is

$$DX\,DY := DX^a\,DY^a\,\delta(x^a x^a + y^a y^a - 1) .$$

Symmetry breaking

As in the spin model, when magnetization takes place, we rotate the Z^a so that only the first component, say Z^1 of Z^a, has a non-zero expectation value. Performing a suitable gauge transformation on the links then leaves $\langle z^1 \rangle = \langle x^1 \rangle$ real. This in turn means the second part of the action (C1.1) contains only cosine terms and hence, $\langle s \rangle$ is also zero.

Thus only h_c and h_x^1 of (1.3) need be considered here. They become (after imposing translation invariance):

$$h_c = 2(d-1)\,\alpha\langle c\rangle^3 + \beta\langle x^1\rangle^2 + J_c \qquad \text{C1.6a}$$

$$h_x^1 = 2d\beta\,\langle c\rangle\langle x^1\rangle + J_x^1 \qquad \text{C1.6b}$$

where self-consistency requires

$$\langle c\rangle = Z_1^{-1} \int D\theta\; c\; \exp\{ch_c\} \qquad \text{C1.7a}$$

$$\langle x^1\rangle = Z_2^{-1} \int DX\,DY\; x^1 \exp\{x^1 h_x^1\} \qquad \text{C1.7b}$$

with
$$Z_1(h) = \int DX\,DY\; \exp\{ch_c\}$$
$$Z_2(h_x^1) = \int DX\,DY \exp\{x^1 h_x^1\} \qquad \text{C1.8}$$

The Legendre transform of the free energy $\omega = \ln Z$ yields the following equation for the thermodynamic potential $\Gamma(\langle c\rangle, \langle x^1\rangle)$:

$$d\Gamma(\langle c\rangle,\langle x'\rangle) = d\,J_c\,d\langle c\rangle + J_x'\,d\langle x'\rangle \qquad \text{C1.9}$$

The solution of equation 4.23 is :

$$\Gamma(\langle c\rangle,\langle x^1\rangle) = \frac{3}{2}\, d(d-1)\, \alpha\langle c\rangle^4 + 2d\, \beta\langle c\rangle\langle x^1\rangle^2$$

$$+ dJ_c\langle c\rangle + J_x^1\langle x^1\rangle - \ln Z_1(h_c) - \ln Z_2(h_x^1) \qquad \text{C1.10}$$

Masses

As in the spin model we consider the responses $\delta\langle c\rangle$ etc. of the average fields to a small source and write down an expression for the change δh_c in the mean fields. Thus ignoring higher derivative terms the Green's functions are obtained.

$$\delta h_c = \alpha \sum_{\substack{3\\4\square 2}} \langle c\rangle^2 [\delta\langle c^2\rangle + \delta\langle c^3\rangle + \delta\langle c^4\rangle$$

$$+ \beta\langle x^1\rangle[\delta\langle x^{1'}\rangle + \delta\langle x^1\rangle] + J_c \qquad \text{C1.11a}$$

$$\delta h_s = \alpha \sum_{\substack{3\\4\square 2\\7\square 5\\6}} \langle c\rangle^2[-\delta\langle s^2\rangle + \delta\langle s^3\rangle + \delta\langle s^4\rangle + \delta\langle s^5\rangle - \delta\langle s^6\rangle]$$

$$+ \beta\langle x^1\rangle[\delta\langle y^1\rangle - \delta\langle y^{1'}\rangle] + J_s \qquad \text{C1.11b}$$

$$\delta h_x^a = \beta \sum_{\longrightarrow x} \langle c\rangle\, \delta\langle x^a\rangle + J_x^a \qquad \text{C1.11c}$$

$$\delta h_y^a = \beta \sum_{\longrightarrow x} \langle c\rangle\, \delta\langle y^a\rangle + J_y^a \qquad \text{C1.11d}$$

where $\langle x^a\rangle = 0$

$$\delta h_x^1 = \beta \sum_{\longrightarrow x} [\langle c\rangle\, \delta\langle x^1\rangle + \langle x^1\rangle\, \delta\langle c\rangle] + J_x^1 \qquad \text{C1.11e}$$

$$\delta h_y^1 = \beta \sum_{\longrightarrow x} \langle c\rangle\, \delta\langle y^1\rangle + \alpha[\sum_{\longrightarrow x}\langle x^1\rangle\, \delta\langle s\rangle - \sum_{x\longrightarrow}\langle x^1\rangle\, \delta\langle s\rangle] + J_y^1 \qquad \text{C1.11f}$$

where $\langle x^1\rangle \neq 0$

Scalar masses

We notice that the expressions for δh^a_x and δh^a_y, where $\langle x^a \rangle = 0$, are essentially identical to that of the Heisenberg model (eqn. 2.23) with $\beta_{HEISENBERG} = \beta \langle c \rangle$. By analogy we call these modes π and we have

$$m_\pi^2 = [\beta \langle c \rangle \langle \pi^a_x \pi^a_x \rangle_c]^{-1} - 2d \qquad \text{C1.12}$$

In the symmetric phases there are $2n$ such degenerate non-zero masses (see Chapter two). In the Higgs phase thaere are $2n-2$ massless Goldstone bosons - the proof is as given for the Heisenberg model in Chapter one, section six .

The value of $\langle \pi^a_x \pi^a_x \rangle_c = \frac{1}{2n}$ found in equation 4.24 is obtained from rotating the $\pi^{a'}_x$ s when symmetry breaking has occurred, i.e.

$$\langle \pi^a_x \pi^a_x \rangle = \langle \sigma_x \sigma_x \rangle = \frac{d}{dh} \langle \sigma \rangle \Big|_{h=0}$$

$$= \frac{h}{dh} \left({}^{I_n}/_{I_{n-1}} \right) \Big|_{h=0}$$

$$\underline{\sim} \; {}^{1}/_{2n} + O(h) \qquad \text{C1.13}$$

'Photon' masses

In the Higgs phase $\delta \langle x^1 \rangle$ mixes with $\delta \langle c \rangle$ and $\delta \langle y^1 \rangle$ with $\delta \langle s \rangle$. For the transverse photons, consider the second case. Writing s^μ_x for the link from site x in direction μ, and Δ_μ for the usual lattice difference operator, equation C1.11b becomes

$$\delta h_{s^\mu_x} = \alpha \langle c \rangle^2 [(\Delta^2 + 2(d-1)) \delta_{\mu\nu} - \Delta_\mu \Delta_\nu] \delta \langle s^\nu_x \rangle$$

$$+ \beta \langle x^1 \rangle \Delta_\mu \delta \langle y^1 \rangle + J_{s^\mu_x} \qquad \text{C1.14}$$

From (C1.11d) we argue that $\delta\langle y^1\rangle$ in (C1.14) mixes with the longitudinal part of $\delta\langle s_x^\mu\rangle$. In addition, the transverse part satisfies $\Delta_\mu \delta\langle s_x^\mu\rangle = 0$. Hence (C1.14) becomes

$$\delta h_{s_x^\mu} = \alpha\langle c\rangle^2 [\Delta^2 + 2(d-1)]\, \delta_{\mu\nu}\, \delta\langle s_x^\mu\rangle + J_{s_x^\mu} \qquad \text{C1.15}$$

Hence we obtain a photon mass m_γ^2 from the equation

$$\delta\langle s_x^\mu\rangle = \langle s_x^\mu\, s_x^\mu\rangle_c\, \delta h_{s_x^\mu} \qquad \text{C1.16}$$

$$= \langle s_x^\mu\, s_x^\mu\rangle_c (\alpha\langle c\rangle^2 [\Delta^2 + 2(d-1)]\, \delta_{\mu\nu})\, \delta\langle s_x^\mu\rangle + J_{s_x^\mu} \qquad \text{C1.17}$$

$$\Longrightarrow \quad (-\Delta^2 + m_\gamma^2)\, \delta\langle s_x^\mu\rangle = \alpha\langle c\rangle^2 J_{s_x^\mu} \qquad \text{C1.18}$$

where

$$m_\gamma^2 = (\alpha\langle c\rangle^2 \langle s_x^\mu\ s_x^\mu\rangle_c)^{-1} - 2(d-1) \qquad \text{C1.19}$$

Using Ward identities as for the Goldstone bosons we now distinguish between transverse photons in the Maxwell and Higgs phases.

Proof C1 : The transverse photons are massless in the Maxwell region.

In this phase $\langle x'\rangle = 0$ and eqn. C1.6a gives

$$\langle s\rangle = Z_1^{-1} \int D\theta \exp\{[2(d-1)\alpha\langle c\rangle^3]c\} \qquad \text{C1.20}$$

Changing variables

$$\delta c = -\varepsilon s \quad , \qquad \delta s = \varepsilon c$$

leads to the Ward identity :

$$0 = \varepsilon(\langle c\rangle - \langle s_x s_x\rangle 2(d-1)\alpha\langle c\rangle^3 + \langle s_x\rangle\langle s_x\rangle 2(d-1)\alpha\langle c\rangle^3) \qquad \text{C1.21}$$

$$= \varepsilon \langle c \rangle \left(1 - \langle s_x \; s_x \rangle_2 (d-1)\, \alpha \langle c \rangle^2\right) \qquad \text{C1.22}$$

$$= \varepsilon \langle c \rangle^3 \; \alpha \; \langle s_x s_x \rangle_c \; m_\gamma^2 \qquad \text{using (C1.19)} \qquad \text{C1.23}$$

$$\Longrightarrow \quad m_\gamma^2 \; = \; 0 \qquad \text{in this phase.}$$

Proof C2 : The photons are massive in the Higgs phase.

Here $\langle x^1 \rangle \neq 0$ and (C1.20) is replaced by

$$\langle S \rangle = Z_1^{-1} \int D\theta \; \exp\{ [2(d-1)\, \alpha \langle c \rangle^3 + \beta \langle x^1 \rangle^2]\theta\} \qquad \text{C1.24}$$

and the Ward identity is :

$$0 = \varepsilon(\langle c \rangle - \langle s_x \, s_x \rangle_c [2(d-1)\; \alpha \; \langle c \rangle^3 + \beta \langle x^1 \rangle^2]) \qquad \text{C1.25}$$

$$= \varepsilon(\langle s_x \, s_x \rangle_c \; \alpha \langle c \rangle^3 \; m_\gamma^2 - \langle s_x \; s_x \rangle_c \; \alpha \langle x^1 \rangle^2) \qquad \text{C1.26}$$

i.e. $$m_\gamma^{2'} = \frac{\beta}{\alpha} \; \frac{\langle x^1 \rangle^2}{\langle c \rangle^3} \qquad \text{(eqn. 4.25)} \qquad \text{C1.27}$$

and it may be shown that m_γ^2 finite persists in the limit $\alpha \to \infty$, β fixed.

PUBLICATIONS

P A P E R 1.

J Phys G: Nucl Phys 7 (1981) L85–L88. Printed in Great Britain

LETTER TO THE EDITOR

The specific heat of SU(3) lattice gauge theory

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Abstract. The average action/plaquette and the specific heat of SU(3) lattice gauge theory in four dimensions are calculated by Monte-Carlo simulation on lattices of lattice length 4 and 5 by averaging over 400 iterations through the 4^4 lattice and 200 iterations through the 5^4 lattice. The calculations show a peak in the specific heat at a value of the inverse temperature β of 6.31.

SU(3) lattice gauge theory in four dimensions is hoped not to possess a phase transition between the low-temperature and the high-temperature regions. This would lead to the confinement of quarks for all values of the temperature (Wilson 1974).

In the present Letter, we evaluate the average action/plaquette $\langle E\rangle$ of SU(3) lattice gauge theory using the Monte-Carlo method (Creutz 1980). The specific heat is then defined by

$$C_V \equiv \partial\langle E\rangle/\partial T = -\beta^2\,\partial\langle E\rangle/\partial\beta \tag{1}$$

where T is the temperature, β is the inverse temperature and $\beta = 6/g^2$, where g is the bare coupling constant. Monte-Carlo calculations have been carried out on lattices of lattice length 4 and 5. For lattice lengths 4 and 5 we used 400 and 200 iterations through the lattice, respectively.

In figure 1 we see the average action/plaquette $\langle E\rangle$ plotted against β, for $0 \leqslant \beta \leqslant 7.0$. (This figure contains 119 data points.) Also shown in the figure are the low-temperature expansion (Creutz 1979)

$$\langle E\rangle \xrightarrow[\beta\to\infty]{} 2/\beta$$

and the high-temperature expansion (Creutz, private communication)

$$\langle E\rangle \xrightarrow[\beta\to 0]{} 1 - \tfrac{1}{18}\beta - \tfrac{1}{216}\beta^2 + \tfrac{5}{93312}\beta^4 + \tfrac{5}{944784}\beta^5 + O(\beta^6).$$

In figure 2 we plot the data for the average action/plaquette shown in figure 1 in the vicinity of the cross-over in order to show the detail more clearly.

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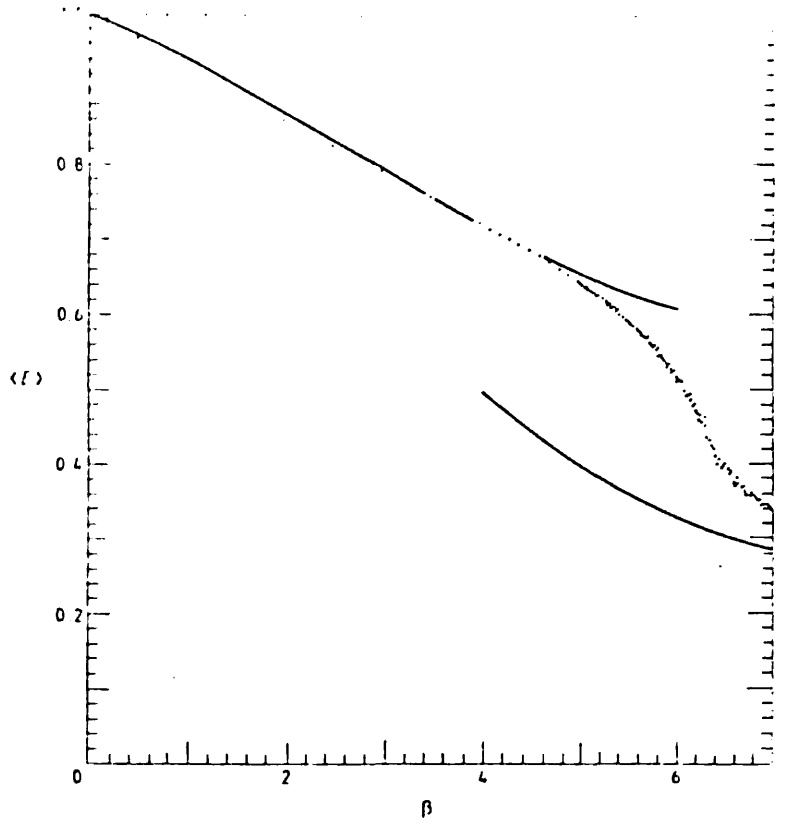

Figure 1. The average action/plaquette for 400 iterations through the lattice for SU(3) lattice gauge theory as a function of the inverse temperature. The low- and high-temperature expansions are also shown.

The specific heat C_V was obtained by first smoothing the average action/plaquette data and then interpolating this smoothed data by means of cubic splines (Anderson *et al* 1979). The cubic spline interpolation then immediately gave the first derivative of the smoothed curve for use in equation (1). We only used ordered (cold start) configurations in our calculations as we know that both ordered (cold start) and disordered (hot start) configurations lead to the same results.

Our results for the specific heat C_V are shown in figure 3. The sharp peak at $\beta \simeq 6.31$ is impressive. This peak occurs near the point ($\beta \simeq 6.00$) where Creutz (private communication) found a rapid cross-over in the string tension between the low- and high-temperature regions. Using the same program, we have computed values of the average action/plaquette for up to $\beta = 15.0$ but this is beyond the transition and thus irrelevant to the present discussion. In the high-temperature region, the agreement between the high-temperature expansion and the Monte-Carlo results is quite good.

We have also evaluated the specific heat for 200 iterations through a 5^4 lattice at 21 values of β. These results indicate that the peak in the specific heat does not shift appreciably in β compared with the 4^4 lattice. This was previously found to be so in SU(2) lattice gauge theory (Lautrup and Nauenberg 1980).

Our results indicate that there is a transition between the low- and high-temperature regions in SU(3) lattice gauge theory, which is similar to that found in SU(2) lattice gauge

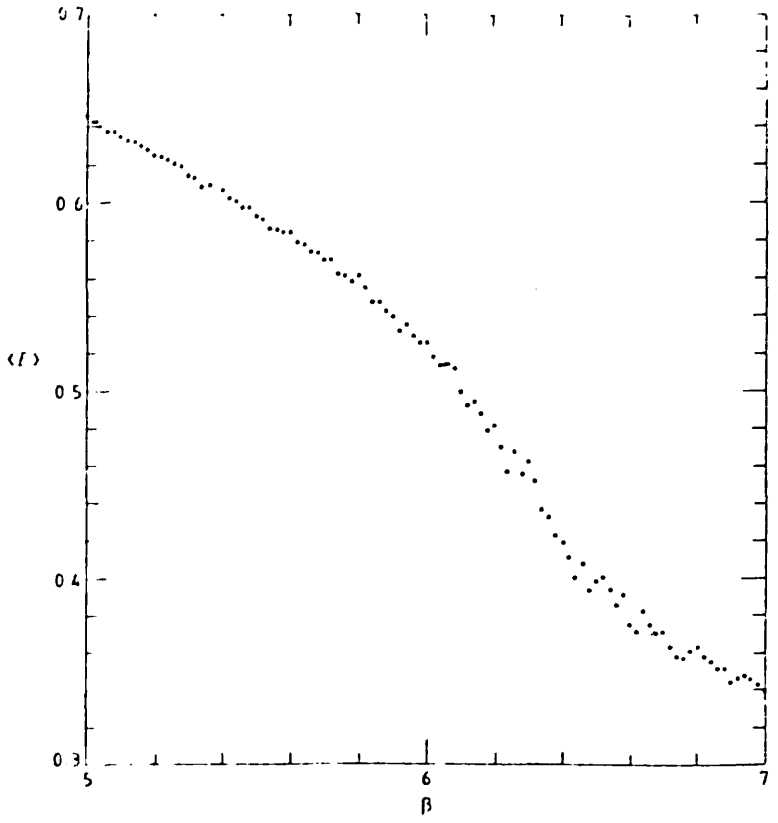

Figure 2. The average action/plaquette for 400 iterations through the lattice for SU(3) lattice gauge theory as a function of the inverse temperature.

theory. In a recent publication, Drouffe and Zuber (1980) found a roughening transition in four-dimensional SU(3) lattice gauge theory at $\beta = 5.94 \pm 0.36$ which corresponds closely with the peak we have found in the specific heat. Using order parameters other than $\langle E \rangle$, such as the pinch operator p_W (Itzykson *et al* 1980), we are continuing to investigate the nature of this phenomenon.

The authors would like to thank Dr M Creutz for his computer program, numerous discussions, correspondence and his constant encouragement, Dr B Lautrup for correspondence concerning his results and Dr M B Green for discussions. Two of the authors (RCE and LMcC) wish to thank the Science Research Council of Great Britain for financial support.

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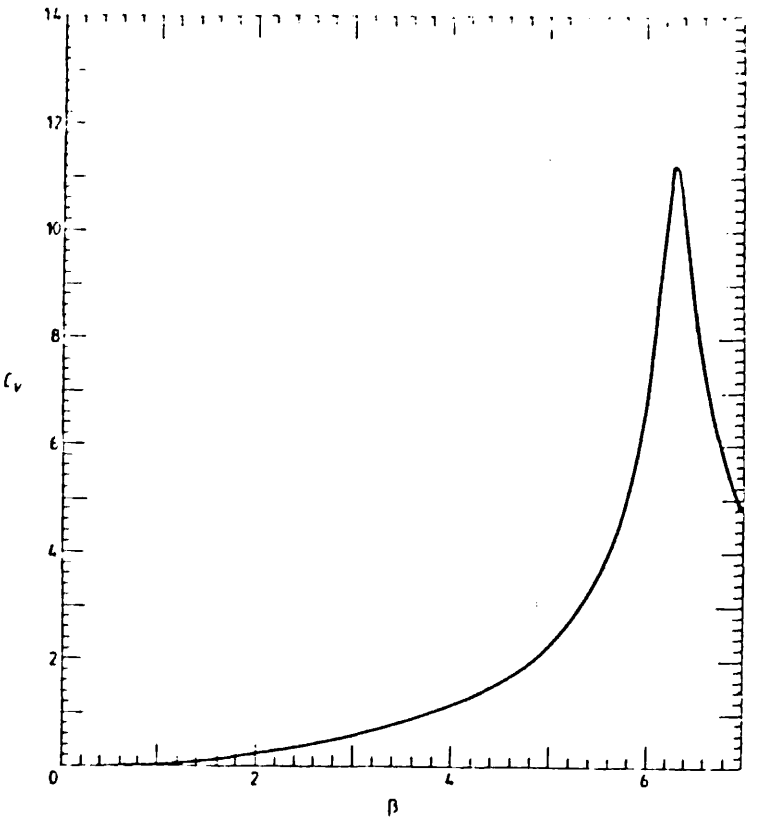

Figure 3. The specific heat C_V for SU(3) lattice gauge theory as a function of the inverse temperature.

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Itzykson C, Peskin M E and Zuber J B 1980 *Phys. Lett.* 95B 259
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PAPER 2.

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MONTE CARLO SIMULATION OF U(1) LATTICE GAUGE THEORY

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PROGRAM SUMMARY

Title of program: U1LATTICE

Catalogue number: ABEA

Program available from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: CDC 7600; *Installation*: ULCC

Operating system: SCOPE

Programming language used: FORTRAN IV

High speed storage required: 16 Kwords

No. of bits in a word: 60

Overlay structure: none

No. of magnetic tapes required: none

Other peripherals used: card reader, line printer

Card punching code: CDC

Total no. of cards in combined program and test deck: 430

Keywords: lattice gauge theory, U(1), quark confinement, phase diagram, phase transition, statistical mechanics, action per plaquette, Monte Carlo

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Nature of the physical problem
The program calculates the average action per plaquette for U(1) lattice gauge theory. Gauge theories formulated on a lattice were proposed by Wilson [1] and Polyakov [2], and the average plaquette action is an important observable in the study of phase transitions in such systems.

Method of solution
A Monte Carlo simulation of the lattice system, using the heat bath method of ref. [3] adapted to U(1), generates a series of field configurations approximating statistical equilibrium at a given temperature.

Restrictions on the complexity of the program
The storage required is dependent on the lattice size. The execution time increases with the lattice size and with the number of Monte Carlo iterations required, and is typically rather long. At temperatures much below the critical point the Monte Carlo vetoing process becomes very slow.

Typical running time
The test run took 34 s on the CDC 7600 at ULCC.

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0010–4655/81/0000–0000/$02.50

LONG WRITE-UP

1. Introduction

The program calculates the average action per plaquette for a U(1) gauge theory on a regular lattice in 2 or more dimensions. Lattice gauge theories are one way of trying to understand gauge-invariant quantum field theories and phenomena such as quark confinement. A popular approach to the investigation of lattice systems is to use the Monte Carlo methodology of numerical simulation which is familiar in statistical mechanics. The algorithm is relatively simple, the main problem being to loop efficiently through the links and their associated plaquettes. It is straightforward for the user to add routines to calculate quantities such as Wilson loops, or to modify the program for groups other than U(1).

2. Outline of the theory

A good introduction to lattice systems with further references is contained in ref. [1]. The lattice is a regular square, cubic or hypercubic array of sites in $n \geqslant 2$ dimensions with l sites on a side. A typical site has integer coordinates $m = (m_1, m_2, ..., m_n)$ where $1 \leqslant m_i \leqslant l$. Nearest neighbour sites i and j are joined by a link which carries an element $U_{ij} = \exp(i\phi_{ij})$ of the group U(1). The links are directed in the sense that $U_{ij} = U_{ji}^{*}$ and

$$\phi_{ij} = \phi_{ji}. \tag{1}$$

Each site carries $2n$ links so that the lattice has $2nl^n$ link variables but (1) reduces the number of independent link angles to nl^n. Periodic boundary conditions are normally applied, neighbours to sites on the edge of the lattice are defined by having:

$$(m_1, ..., m_i + l, ..., m_n) \equiv (m_1, ..., m_i, ..., m_n). \tag{2}$$

In other words, the lattice repeats in every direction.

A plaquette is a square of nearest-neighbour sites in a lattice plane which we label $(ijkl)$ (fig. 1). The action for this typical plaquette p is

$$S_p = 1 - \mathrm{Re}(U_{ij} U_{jk} U_{kl} U_{li}),$$

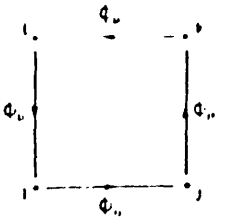

Fig. 1. A plaquette of the lattice.

or

$$S_p = 1 - \cos(\phi_{ij} + \phi_{jk} + \phi_{kl} + \phi_{li}), \tag{3}$$

and the total action for the system in a configuration C is

$$S_C = \sum_p S_p,$$

where each combination $(ijkl)$ is counted only once. If different permutations $(ilkj)$, $(klij)$, etc. are counted separately, there is also a factor $\frac{1}{8}$. The partition function is

$$Z = \sum_C \exp\{-\beta S_C\},$$

where the sum stands symbolically for an integration over all possible configurations. The parameter β is known as the inverse temperature and corresponds to the inverse coupling constant squared in field theory. If the continuum limit is correctly taken, the link angle $\phi_\mu(m)$ can be identified with the electromagnetic field $A_\mu(x)$; $\phi_\mu(m)$ denotes the angle on the link from the site with coordinates m in the μ direction. Then the action becomes

$$S = \tfrac{1}{4} \int d^4x \, (\partial_\mu A_\nu - \partial_\nu A_\mu)(\partial_\mu A_\nu - \partial_\nu A_\mu),$$

which is the usual Euclidean action for the electromagnetic field.

3. Monte Carlo method

The theory and practice of the Monte Carlo technique is comprehensively discussed in ref. [2]. At values of β far from a critical region, the lattice configuration converges very rapidly to a stable state

with relatively small thermal fluctuations, whatever the initial state. Near a critical value of β, however, convergence will be slower and the variations of larger amplitude. If insufficient iterations are made, hysteresis effects will be apparent.

4. The program

A description of the program and its use is included in comment cards. There are two subroutines: CHECK, which traps illegal values of parameters that the user may alter; and SWEEP which performs a single Monte Carlo sweep through all the links on the lattice and returns the average plaquette action. The main program initialises the lattice to an ordered configuration ($\phi_{ij} = 0$) or to a disordered configuration (ϕ_{ij} selected at random in the range $[0, 2\pi]$), and calls SWEEP repeatedly. The main program also includes assignment statements for parameters controlling the Monte Carlo process and for β, n, l. To run the program, the user alters these assignments as he wishes and adjusts the dimensions of arrays storing lattice variables accordingly (this is explained in more detail by comments). The program calls NAG routine G05CAF [3] which returns a random number uniformly distributed between 0 and 1, but any similar function could be substituted. The main program and CHECK are easily understood, so we now concentrate on the subroutine SWEEP. It is necessary to loop through each link in turn, calculating the action around each plaquette which includes that link.

At the site with coordinates m_i there are n links in the positive directions, and the values of $\cos \phi_{ij}$ and $\sin \phi_{ij}$ on these links are stored in the arrays COSP and SINP, respectively. The link in the positive k direction from this site is at location

$$k + n \sum_{i=1}^{n} (m_i - 1) l^{i-1} \qquad (4)$$

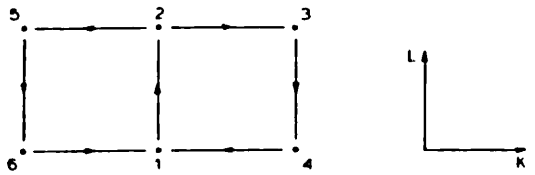

Fig. 2. The two plaquettes in the K, L plane.

in these arrays. The coordinate m_i is at location i in array ICOORD.

Given the link in the L direction from a site (which is denoted 1) there are two plaquettes to be considered in the K, L plane (fig. 2), which we denote (1234) and (1256). Site 1, with coordinates m_i, has an entry in COSP and SINP starting at location

$$\text{NSITE1} = 1 + n \sum_{i=1}^{n} (m_i - 1) l^{i-1}$$

and similarly for NSITE2, NSITE5 and NSITE6. The values of $\cos \phi_{12}$ and $\sin \phi_{12}$ will be at location

$$\text{LINK12} = L + n \sum_{i=1}^{n} (m_i - 1) l^{i-1}$$

$$= \text{NSITE1} + (L - 1).$$

To save explicitly evaluating the sums of (4), it is possible to simply find the displacement in COSP and SINP caused by moving to a neighbouring site in a given direction. To move one site in the $\pm k$ direction, i.e. to the site with coordinates

$$m_i' = m_i \pm \delta_{ik},$$

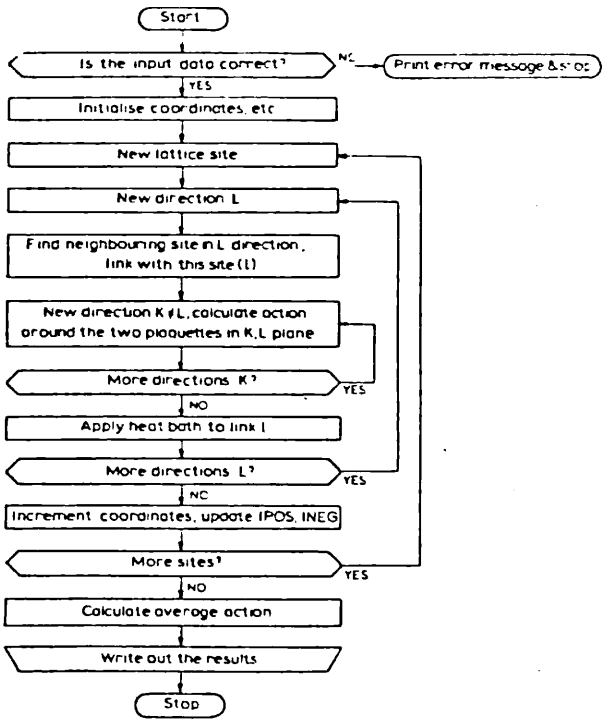

Fig. 3. Flowchart summarising the program, carrying out one sweep.

it can be seen from (4) that the displacement is $-nl^{k-1}$.

The periodic boundary conditions result in special cases when m is at the beginning or end of a row in the k direction. Using (2) we see that

a) when $m_k = 1$ to move one site in the $-k$ direction $(l-1)nl^{k-1}$ must be added; and

b) when $m_k = l$ to move one site in the $+k$ direction $(1-l)nl^{k-1}$ must be added.

The pointer arrays INCPOS and INCNEG are set to:

$$\mathrm{INCPOS}(k) = nl^{k-1}, \quad \mathrm{INCNEG}(k) = (1-l)nl^{k-1}.$$

The arrays IPOS and INEG are maintained so that to move one step in the $+k$ direction IPOS(k) has to be added, and to move one step in the $-k$ direction INEG(k) has to be added. Normally, then, IPOS(k) = INCPOS(k) and INEG(k) = $-$INCPOS(k); but if $m_k = 1$ then INEG(k) = $-$INCNEG(k) and if $m_k = l$ then IPOS(k) = INCNEG(k). Using these pointers it is now easy to locate the values of $\cos\phi_{ij}$ and $\sin\phi_{ij}$ around the two plaquettes of fig. 2.

The output from the program is self-explanatory. The test run output will only be approximately reproduced by the user because of the dependence on the random number generation. The flowchart of the program is shown in fig. 3.

Acknowledgements

One of the authors (K.J.M.M.) wishes to thank Dr. E. Pietarinen for initiating his interest in lattice gauge theory, for many fruitful discussions and for showing him how to carry out Monte Carlo simulation of a lattice gauge theory on a computer, Professor G. Mack and Dr. B. Berg for numerous discussions, and finally the DESY directorate for the award of a Visiting Fellowship to visit DESY where this work was begun. Two of the authors (R.C.E. and L.McC.) wish to thank the Science Research Council of Great Britain for financial support.

References

[1] J.B. Kogut, Rev. Mod. Phys. 51 (1979) 659.

[2] Monte Carlo methods in statistical physics, ed. K. Binder (Springer Verlag, Berlin, 1979).

[3] NAG Mark 7 FORTRAN Library Manual, available from Numerical Algorithms Group, 7 Banbury Rd., Oxford, England.

TEST RUN OUTPUT

```
MONTE-CARLO SIMULATION OF U(1) LATTICE THEORY
*********************************************

ACTION PER PLAQUETTE

LATTICE IS  4 WIDE BY 4 HIGH  4 SITES
TOTAL NUMBER OF SWEEPS        500
ORDERED INITIAL CONFIGURATION
INVERSE TEMPERATURE (BETA)    .5000000E+01
```

SWEEP	ACTION/PLAQ	SWEEP	ACTION/PLAQ	SWEEP	ACTION/PLAQ	SWEEP	ACTION/PLAQ	SWEEP	ACTION/PLAQ
10	.76743E+00	20	.75810E+00	30	.75543E+00	40	.75547E+00	50	.76744E+00
60	.76153E+00	70	.76017E+00	80	.76841E+00	90	.73797E+00	100	.75554E+00
110	.74936E+00	120	.74936E+00	130	.73903E+00	140	.76838E+00	150	.78560E+00
160	.73531E+00	170	.75926E+00	180	.77712E+00	190	.77370E+00	200	.73900E+00
210	.75151E+00	220	.74047E+00	230	.72839E+00	240	.77240E+00	250	.77720E+00
260	.75955E+00	270	.76376E+00	280	.77352E+00	290	.75084E+00	300	.75607E+00
310	.74935E+00	320	.76422E+00	330	.74514E+00	340	.76767E+00	350	.76295E+00
360	.75944E+00	370	.75152E+00	380	.73443E+00	390	.76244E+00	400	.75316E+00
410	.75685E+00	420	.76366E+00	430	.76653E+00	440	.75641E+00	450	.76825E+00
460	.77367E+00	470	.74900E+00	480	.75092E+00	490	.73874E+00	500	.75712E+00

AVERAGE OVER ALL 500 SWEEPS .75436E+00

AVERAGE OVER LAST 450 SWEEPS .75508E+00

PAPER 3.

CP^{N-1} COUPLED TO GAUGE FIELDS: MEAN FIELD THEORY AND MONTE CARLO RESULTS

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We define a two parameter lattice field theory which interpolates between the O(2N) Heisenberg model, pure U(1) gauge theory, and a lattice version of the CP^{N-1} model. The phase diagram in space–time dimension $d = 4$ is obtained by Monte Carlo simulation on a 4^4 lattice, and the nature of the phases is discussed in mean field approximation.

General features of the phase diagrams for lattice formulations of various Higgs models (coupled spin-gauge systems) have been understood both by qualitative theoretical arguments and by numerical simulation (refs. [1–7]). In these models the scalar fields (defined on the lattice sites) have fixed length and are able to give a mass to some of or all of the gauge fields by the Higgs mechanism, depending on their number and in which representation of the gauge group they lie.

In this letter we extend such investigations to models in which there are more site spins (each in the fundamental representation) than are necessary to break the gauge symmetry completely. For simplicity we restrict our attention to systems having an abelian gauge group U(1): these include the CP^{N-1} models (refs. [8,9]) as special limits. We are partially motivated by the wish to understand suggested connections between the continuum field theories of CP^{N-1} and N-component scalar QED (ref. [10]).

The theories we consider are defined by the euclidean lattice action density

$$S_i = -\frac{\alpha}{2}\sum_{\substack{\mu,\nu \\ \mu>\nu}} U_{i,\mu}U_{i+\hat{\mu},\nu}\bar{U}_{i+\hat{\nu},\mu}\bar{U}_{i,\nu} - \frac{\beta}{2}\sum_{\mu,a} z_a(i)\,U_{i,\mu}z_a(i+\hat{\mu}) + \text{c.c.}\,, \tag{1}$$

where the spin $z_a(i)$ at site i is a set of N complex scalar fields ($N > 1$) in the fundamental representation of the global symmetry group U(N) as well as the local U(1). It satisfies the fixed length condition

$$\sum_a \bar{z}_a(i) z_a(i) = 1\,.$$

The variable $U_{i,\mu}$ is a complex phase factor defined on the link between sites i and $i+\hat{\mu}$, $\hat{\mu}$ being a unit lattice vector in d dimensions: we shall take d to be 4. Thus the action

$$S = \sum_i S_i \equiv \alpha \sum_{\mathrm{p}} P_{\mathrm{p}} + \beta \sum_{\ell} L_{\ell} \tag{2}$$

is the sum over plaquettes p of the usual Wilson action P_{p} with coupling α, plus the sum over links ℓ of the simplest gauge invariant nearest-neighbour spin–spin interaction L_{ℓ}, coupling β.

The partition function is defined as

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$$Z = \sum_{\{z,\bar{z},U\}} \exp(-S) , \tag{3}$$

and simplifies in the various extreme limits of α,β:

(a) $\beta \to 0$. The spin integration is trivial, and the model becomes pure U(1) gauge theory, which is known in $d = 4$ to have a second order transition between confining and Maxwell phases. Integrating out the spin degrees of freedom for non-zero β introduces extra (gauge invariant) interactions of the link variables. The first contribution occurs at $O(\beta^4)$ and amounts to an additive renormalization of α by $+\beta^4/8N^3$. Thus we expect the transition point in the pure U(1) gauge theory to lie at the end of a line of transitions given by

$$\alpha_c(\beta) = \alpha_c(0) - \beta^4/8N^3 + O(\beta^6) ,$$

but cannot rule out the possibility that the transition goes first order.

(b) $\beta \to \infty$. In this limit the configurations that minimize L in (1) have the spins frozen into a state of complete "magnetization". Following ref. [11] this may be characterized in a gauge invariant manner as the state in which the matrix order parameter

$$Q_{ab} = \bar{z}_a(i) z_b(i) - N^{-1}\delta_{ab}$$

attains its maximal value, diag$[1 - 1/N, -1/N, ..., -1/N]$. Furthermore the link variables must be in a pure gauge configuration to minimize L. Thus there is no α-dependence and the model is trivial.

(c) $\alpha \to 0$. This limit is non-trivial for $N > 1$, in contrast to the case $N = 1$ considered in ref. [4]. The integrations over link variables factorize, giving

$$\begin{aligned} Z &= \int \mathcal{D}\bar{z}\, \mathcal{D}z \prod_{i,\mu} \int_0^{2\pi} d\theta \\ &\quad \times \exp(\beta |\bar{z}(i)\cdot z(i+\hat{\mu})| \cos\theta) \\ &= \int \mathcal{D}\bar{z}\, \mathcal{D}z \exp\Big(\sum_{i,\mu} \ln I_0 \\ &\quad \times (\beta |\bar{z}(i)\cdot z(i+\hat{\mu})| \;) \Big) . \end{aligned} \tag{4}$$

This is a lattice version of the CP^{N-1} model (an alternative to that discussed in ref. [12]). In terms of the gauge invariant projectors $P_{ab}(i) = \bar{z}_a(i) z_b(i)$, the action in eq. (4) reads

$$\frac{\beta^2}{4} \sum_{i,\mu} \mathrm{tr}\, P(i) P(i+\hat{\mu}) - \frac{\beta^4}{64} \sum_{i,\mu} [\mathrm{tr}\, P(i)\, P(i+\hat{\mu})]^2 + ... ,$$

and, by analogy with the results of ref. [11], the phase transition between order ($\beta = \infty$) and disorder ($\beta = 0$) might be expected to be first order, except for $N = 2$, and possibly other low values of N.

(d) $\alpha \to \infty$. The link variables are forced in this limit into pure gauge configurations. In the gauge where all links are 1, the action reduces to the $O(2N)$ Heisenberg model. Thus the partition function (3) becomes an integral over all gauge transformations of that for the Heisenberg model, and should have the same phase transition. However singularities will occur only in the gauge invariant quantities like $\langle Q_{ab} \rangle$, and not in $\langle z_a \rangle$, which always vanishes.

We have obtained the phase diagram of the model for finite and positive values of the couplings α, β, by Monte Carlo simulation on a 4^4 lattice, for $N = 2, 3$. By using an algorithm analogous to that of Metropolis et al. (ref. [12]), we generated sequences of configurations of spin and gauge degrees of freedom, obeying the equilibrium distribution, for various values of α, β. From these we extracted values for the two terms contributing to the action (1)

$$\langle P \rangle \equiv \tfrac{1}{2} \langle U_{i,\mu} U_{i+\hat{\mu},\nu} \bar{U}_{i+\hat{\nu},\mu} \bar{U}_{i,\nu} + \text{c.c.} \rangle ,$$

$$\langle L \rangle = \tfrac{1}{2} \langle \bar{z}(i) \cdot U_{i,\mu} z(i+\hat{\mu}) + \text{c.c.} \rangle ,$$

averaged over all positions and orientations on the lattice. In the behaviour of these expectation values over a "thermal" cycle involving some variation of α, β, possible phase transitions show up as regions of poor convergence, i.e. hysteresis loops. The results are displayed in figs. 1, 2, where the length of the bars indicate roughly the extent of the hysteresis loops.

Combining the results for $\langle P \rangle$ and $\langle L \rangle$, we find evidence for three phases in each model but cannot be sure what order the various transitions are. As shown in fig. 3, we find that the transitions tend to show up more clearly in one expectation value than the other. In the mean field analysis presented below, each transition is associated with the ordering of one or both types of degree of freedom. Thus it is not surprising that the spin ordering transition (B) is visible in $\langle L \rangle$ but not $\langle P \rangle$ and likewise the gauge ordering transition (A) shows in $\langle P \rangle$, not $\langle L \rangle$. However a more direct argument can be given, assuming the free energy density $\Gamma^{(i)}$ to be analytic within each phase ($i = 1, 2$) so that

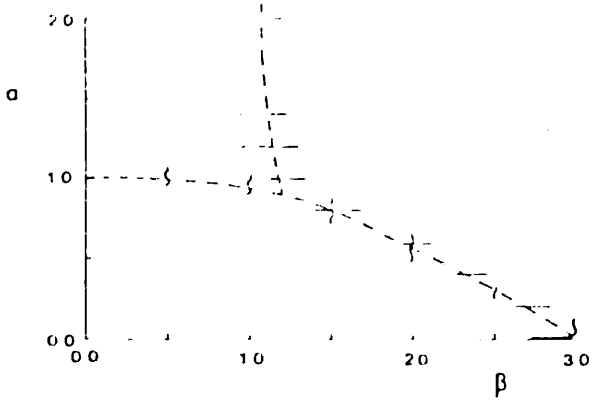

Fig. 1. Phase diagram for CP^2 coupled to gauge fields, obtained by Monte Carlo simulation of 4^4 lattice. Horizontal and vertical bars indicate regions of slow convergence of $\langle L\rangle$, $\langle P\rangle$ respectively.

$$d\Gamma^{(i)} = (\partial\Gamma^{(i)}/\partial\alpha)d\alpha + (\partial\Gamma^{(i)}/\partial\beta)d\beta$$

$$= \tfrac{1}{2}(d-1)\langle P\rangle^{(i)}d\alpha + \langle L\rangle^{(i)}d\beta\,.$$

For a first order transition between phases (1) and (2) the coexistence curve satisfies $d\Gamma^{(1)} = d\Gamma^{(2)}$, i.e.

$$\tfrac{1}{2}(d-1)(\langle P\rangle^{(1)} - \langle P\rangle^{(2)})d\alpha$$

$$= (\langle L\rangle^{(2)} - \langle L\rangle^{(1)})d\beta\,,$$

$$d\alpha/d\beta = [-2/(d-1)]\,\Delta\langle L\rangle/\Delta\langle P\rangle\,. \qquad (5)$$

(This is just Clapeyron's equation.) Thus the ratio of discontinuities in $\langle L\rangle$ and $\langle P\rangle$ is trivially determined by the orientation of the phase boundary in the α–β plane.

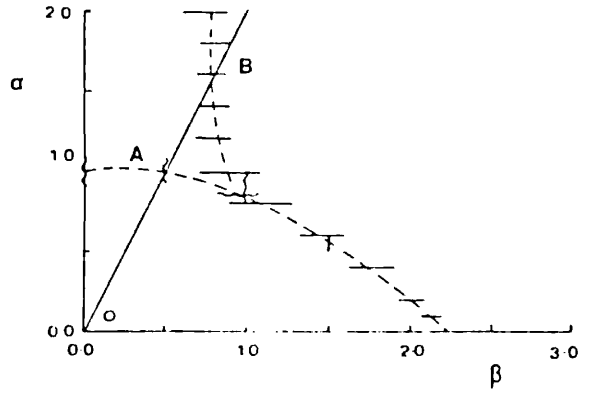

Fig. 2. As fig. 1 but CP^1 coupled to gauge fields. The line OAB indicates the path of the thermal cycle plotted in fig. 3.

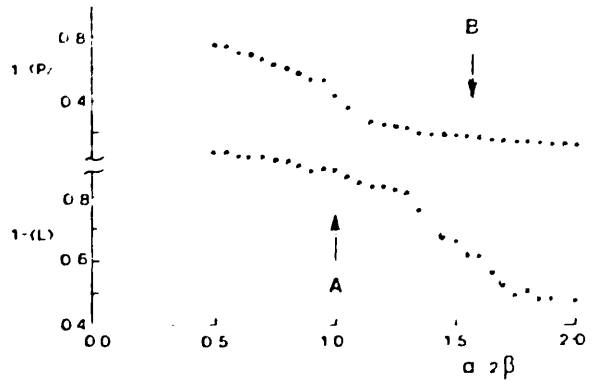

Fig. 3. Thermal cycle obtained in CP^1 coupled to gauge fields for the line $\alpha = 2\beta$ in fig. 2, showing different behaviour of $\langle L\rangle$ and $\langle P\rangle$.

In particular, the slope of the phase boundary must always be negative since $\langle L\rangle$ and $\langle P\rangle$ are essentially specific heats, and therefore both positive. At higher order transitions, which may have non-classical critical exponents, the right-hand side of eq. (5) is replaced by the ratio of the amplitudes of the leading singularity in $\langle L\rangle$, $\langle P\rangle$. Presumably these amplitudes determine the relative extent to which the phase transition shows up via hysteresis loops in any Monte Carlo simulation.

To extract some of the physics in each phase, we consider the mean field approximation, in which each degree of freedom is taken to interact with the average value of its neighbours. This decouples the integrals in eq. (3) and leads to a pair of self consistency conditions on the site and link expectation values, which we assume are spatially uniform. We use the remaining unbroken symmetries to rotate $\langle z_a\rangle$ to that only $\langle z_n\rangle$ may be nonzero, and make $\langle U\rangle \equiv c$, $\langle z_n\rangle \equiv x$ both real. In terms of the corresponding mean fields

$$h_c = 2(d-1)\alpha c^3 + \beta x^2\,, \quad h_x = 2d\beta c x\,, \qquad (6)$$

and defining

$$\omega_n(h) = \ln\left(\int d^{2n}\phi\,\delta(1-\phi^2)\exp(h\phi_{2n})\right)$$

the self consistency conditions are

$$x = \omega_N'(h_x) = I_N(h_x)/I_{N-1}(h_x)\,,$$

$$c = \omega_1'(h_c) = I_1(h_c)/I_0(h_c)\,. \qquad (7)$$

We have ignored the apparent inconsistency with Elitzur's theorem, which requires that both x and c

vanish. This could be removed by choosing a gauge. For instance in an axial gauge the mean fields become

$$h_\lambda^{\text{axial}} = 2\beta[(d-1)c+1]x\,,$$

$$h_c^{\text{axial}} = 2\alpha[(d-2)c^3+c]+\beta x^2\,,$$

and lead to a qualitatively identical phase diagram for $d = 4$, ref. [1].

Any ambiguity in the solution of eqs. (7) is removed by minimizing the free energy Γ, which turns out in this approximation to be

$$\Gamma_{\text{MF}} = -\tfrac{1}{2}\alpha d(d-1)c^4 - \beta dcx^2 + \gamma_N(x) + \mathrm{d}\gamma_1(c)\,,$$

per site, where γ_n is the Legendre transform of ω_n. The resulting phase diagram for $N = 3$ is shown in fig. 4, which is to be compared with the Monte Carlo results, fig. 1. The names given to the phases in fig. 4 are justified by calculating the mass spectrum in each. We omit the details, which are rather tedious, merely outlining the method, which is standard. Position-dependent source terms are introduced into the action, one for each field, so that the expectation values $\langle z\rangle$, $\langle \bar{z}\rangle$, $\langle U\rangle$ become position dependent too. Re-expressing the free energy Γ_{MF} in terms of the momentum space components of the fields, $\tilde{x}(p_\mu)$, etc., and letting $p^2 \to 0$ allows one to read off the masses from the quadratic part of Γ_{MF}, so, for example

$$\Gamma_{\text{MF}}(o) = [A + Bp^2 + O(p^4)]\,o(p)o(-p) + \ldots$$

$$\to m_o^2 = A/B\,.$$

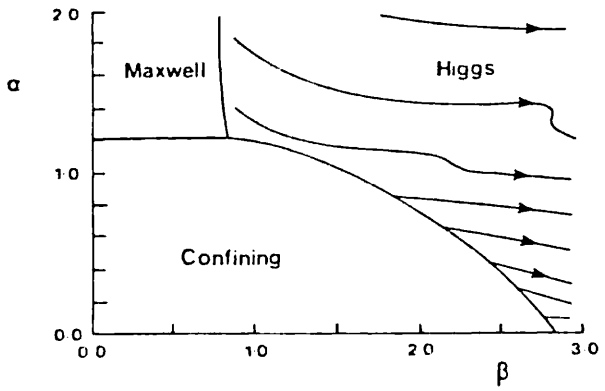

Fig. 4. Phase diagram for CP^2 coupled to gauge fields, obtained in mean field approximation. The flow indicated in the Higgs phase is in the direction of increasing m_σ^2, keeping m_γ^2/m_σ^2 fixed.

The results are as follows:

(i) In the small-α, small-β phase, $c = 0$, and all masses are infinite since neighbouring degrees of freedom decouple, making all correlation lengths vanish. Thus the charged fields z_a are confined, albeit for trivial reasons: the would-be bound states Q_{ab} also have infinite mass in this simplest mean field analysis.

(ii) In the large-α, small-β phase, the spin fluctuations correspond to a degenerate set of $2N$ massive scalars

$$m_{z,\bar{z}}^2 = 2N/c\beta - 2d \quad (\beta \leqslant \beta_c = N/dc)\,.$$

There are $2d$ modes of fluctuation in the link $\langle U_\mu\rangle$. $2d-1$ are transverse to $\langle U_\mu\rangle_{p^2=0}$, and one longitudinal. The longitudinal mode, and $d-1$ of the transverse modes are massive and irrelevant, since the mass remains non-zero in the continuum limit $m_{z,\bar{z}}^2 \to 0$ (in units of the lattice cutoff), i.e. $\beta \to \beta_c$. Of the remaining d massless transverse modes, one is the unphysical gauge degree of freedom, and the other $d-1$ are the photon, whose longitudinal polarization decouples when $\beta \to \beta_c$.

(iii) In the third phase, the Higgs mechanism occurs. There remain $2(N-1)$ massless Goldstone bosons:

$$m_\pi^2 = (c\beta\langle\pi\pi\rangle_c)^{-1} - 2d = 0\,,$$

which follows from the Ward identity

$$x - \langle\pi\pi\rangle_c\, x\, 2dc\beta = 0\,,$$

since $x \neq 0$. The photon is massive

$$m_\gamma^2 = (\beta/\alpha)\,x^2/c^3 > 0$$

having $d-1$ polarizations. Just one more degree of freedom is physical, the massive scalar field o. The calculation of its mass is complicated by mixing between $\langle z\rangle$ and the longitudinal mode in $\langle U_\mu\rangle$. The physical o is identified with the state having the lower mass, which tends to zero as $\beta \to \beta_c$. We omit the rather complicated formula for m_o^2, and instead have plotted in fig. 4 contours along which the ratio of the two physical masses m_γ and m_o are constant.

The existence in this two coupling constant model of two physical masses allows us to define (at least in the Higgs phase) a phenomenological renormalization group, as follows. We require the couplings α and β to depend on the lattice cutoff Λ in such a way that both m_γ^2 and m_o^2 remain constant as Λ varies. Thus

$$m_\gamma^2(\alpha,\beta) = f(\alpha,\beta)\Lambda^2\,, \quad m_o^2(\alpha,\beta) = g(\alpha,\beta)\Lambda^2\,.$$

$$\frac{d\alpha}{d\ln\Lambda^2} = \left(f\frac{\partial r}{\partial\beta} - r\frac{\partial f}{\partial\beta}\right)\Big/\left(\frac{\partial f}{\partial\alpha}\frac{\partial r}{\partial\beta} - \frac{\partial r}{\partial\alpha}\frac{\partial f}{\partial\beta}\right),$$

for instance, and the speed of the resulting flow tends to zero with f, g at a second order transition. In the mean field approximation, this flow will be along the contours plotted in fig. 4. Quantum corrections to this mean field picture will modify this flow, however we have not attempted to calculate them.

Ref. [13] includes the results of a one-loop calculation for the corresponding continuum field theory, of charged scalars interacting with photons. Perturbing in the gauge coupling e^2 and in the scalar interaction $\lambda(\phi^*\cdot\phi)^2$, they find for $N \leq 365$ a first order transition separating Higgs and Maxwell phases, and an infrared instability in $e^2 = 1/\alpha$ at the fixed point $\alpha = \infty$, $\beta = \beta_c$, $\lambda = 0$. Thus one might expect that the Higgs/Maxwell phase boundary in the lattice theory considered here is also first order, if these results persist in the limit $\lambda_{BARE} \to \infty$ required to impose the constraint on the length of the scalar field.

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