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MONTE CARLO SIMULATION OF THE MASSIVE SCHWINGER MODEL

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A B S T R A C T

In this article we apply a previously proposed deformationization method to the study of two-dimensional QED (massive Schwinger model). We find good evidence for the spontaneous breaking of axial symmetry, i.e., $\langle \bar{\psi}\psi \rangle \neq 0$ in the massless limit.

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1. - INTRODUCTION

Monte Carlo methods have proved very powerful in the study of quantum gauge theories ¹⁾. In order to apply them to fully realistic situations, fermions must be introduced into the algorithm. The straightforward introduction of anti-commuting variables is impossible. It was, however, suggested in Ref. 2) that one could integrate the fermionic degrees of freedom by the Matthews-Salam formula ³⁾ and then perform the bosonic integral using standard Monte Carlo techniques. Unfortunately, if the degrees of freedom of the system are N , the analytic evaluation of the fermionic determinant involves N^3 terms so that the algorithm is slowed down by a factor of N^3 : the method cannot be used unless N is very small. As was stressed in Ref. 2), the real problem consists of finding a fast algorithm to evaluate the determinant (or, even better, the ratio of two determinants). As far as Monte Carlo methods are concerned, one only needs an approximate estimate of the determinant. It was then suggested that the ratio of the determinants be computed by a Monte Carlo simulation over bosonic variables (which will be called pseudofermions). In this way, irrespective of the number of dynamical variables N , the time spent in the algorithm is only increased by a factor of n , n being the number of pseudofermionic iterations needed to achieve, within the desired accuracy, statistical equilibrium of the pseudofermions. Simulations of simple systems have indicated that the error in this method is proportional to $1/n$. The estimate of the magnitude of the error is obtained by considering the associated Langevin equation ⁴⁾.

Before applying our technique to four-dimensional gauge theories, we decided to test it by studying a simplified model ; we have chosen this to be two-dimensional QED ⁵⁾⁻¹⁰⁾, or massive Schwinger model, for which several analytic results are available. We report here on the outcome of our computations.

In Section 2 we formulate the lattice action, in the form most convenient for our method, and we discuss how spontaneous breaking of axial symmetry should manifest itself in the massless limit. In Section 3 we study the system, neglecting fermionic induced vacuum polarization diagrams (the quenched case). The case in which $\beta \equiv 1/g^2 \rightarrow -\infty$ can be solved analytically and, in this case, axial symmetry is spontaneously broken. In Section 4 we analyze the quenched case by Monte Carlo computations. In Section 5 we explain how the Monte Carlo procedure is extended to take into account fermionic vacuum polarization (annealed case, in metallurgic terminology). As a test of the procedure, the results for a 2×2 lattice are obtained and compared with the method based on the exact evaluation of the

determinant. Finally, in Section 6 we present our results for a 16×16 lattice, for various values of the fermionic mass, at $\beta = 3$. Our conclusions are drawn in Section 7.

2. - THE LATTICE ACTION

We need a lattice formulation of the Euclidean action :

$$S = \int d^2x \left\{ \bar{\psi} (\gamma^\mu D_\mu + m) \psi + \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right\}, \quad (2.1)$$

where $\psi, \bar{\psi}$ are two-component spinors and D_μ stands for the covariant derivative $\partial_\mu + igA_\mu$. Lattice models with fermions are plagued with a proliferation of modes, the cause of which can be explained in various ways¹¹⁾, but which are all eventually related to the presence of first order derivatives. On a lattice, a derivative like $\partial_x \psi$ will be approximated, unless one wants to introduce asymmetries and possible non-Hermiticities, by a central difference :

$$\partial_x \psi \approx \frac{\psi(x+a) - \psi(x-a)}{2a}, \quad (2.2)$$

a being the lattice spacing. This effectively makes $2a$ the size of the unit cell, and the values of the field at the 2^d (d being the dimensionality) points inside the cell turn up as additional degrees of freedom.

An ingenious way of alleviating the problem is the one proposed by Susskind¹²⁾, namely assigning single components of the spinors, rather than the full spinors, to the various lattice points inside the cell. In a two-dimensional Euclidean system the formulation becomes particularly elegant if one uses a representation

$$\gamma_1 = \sigma_1, \quad \gamma_2 = \sigma_2, \quad \gamma_5 = -i\gamma_1\gamma_2 = \sigma_3 \quad (2.3)$$

for the Dirac matrices, so that ψ^+ and ψ^- , the upper and lower components of ψ , are chirality eigenstates. Then, denoting the points of a square lattice by integers i and j , the one-component variables ψ_{ij} with $i+j$ even and odd, respectively, can be conveniently taken to represent the fields ψ^+ and ψ^- .

The free lattice action takes the form

$$S = \sum_{ij} \left\{ \bar{\psi}_{ij} (\psi_{i+1j} - \psi_{i-1j}) - \right. \\ \left. - i(-1)^{i+j} \bar{\psi}_{ij} (\psi_{ij+1} - \psi_{ij-1}) + \mu \bar{\psi}_{ij} \psi_{ij} \right\}. \quad (2.4)$$

(In this formula, as we shall often do in the following, we set $a = 1$, or equivalently, the lattice spacing may be thought of as absorbed in a rescaling of ψ .) Notice that the $\gamma^1 \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ matrix of the continuum action manifests itself simply in the fact that the first term in Eq. (2.4) couples sites of different "chirality", whereas the factor $-i(-1)^{i+j}$ reproduces the alternation of signs of $\gamma^2 \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$.

To couple in a $U(1)$ gauge field is straightforward : one just follows the standard formulation of lattice gauge theories. Group elements U_{ij}^x and U_{ij}^y (of the form $e^{i\theta}$) are associated with the links between sites ij and $i+1j$, $ij+1$, respectively, and are used for the covariant transport of the complex fields between neighbouring sites (the reversed transports $i+1j \rightarrow ij$, $ij+1 \rightarrow ij$ being of course performed by $\bar{U}_{ij}^x$ and $\bar{U}_{ij}^y$). The fermionic part of the action then becomes :

$$S_F = (\bar{\psi}, G(U)\psi) \equiv \\ \equiv \sum_{ij} \left\{ \bar{\psi}_{ij} \bar{U}_{ij}^x \psi_{i+1j} - \bar{\psi}_{ij} U_{i-1j}^x \psi_{i-1j} - \right. \\ \left. - i(-1)^{i+j} (\bar{\psi}_{ij} \bar{U}_{ij}^y \psi_{ij+1} - \bar{\psi}_{ij} U_{ij-1}^y \psi_{ij-1}) + \mu \bar{\psi}_{ij} \psi_{ij} \right\}. \quad (2.5)$$

The pure gauge part of the action is given by

$$S_G = \beta \sum_{\square ij} (1 - \text{Re } U_{\square ij}), \quad (2.6)$$

where the sum is extended to all elementary squares of the lattice (plaquettes) and

$$U_{\square ij} = U_{ij}^x U_{i+1j}^y \bar{U}_{ij+1}^x \bar{U}_{ij}^y. \quad (2.7)$$

The relation between the coupling constant g , the lattice spacing a and the parameter β in Eq. (2.6) is given by

$$\beta = \frac{1}{g^2 a^2}. \quad (2.8)$$

Indeed, writing

$$U_{ij}^\mu = \exp \{ i g a A_\mu(ia, ja) \},$$

the lattice gauge action reduces in the $a \rightarrow 0$ limit to the familiar form $\frac{1}{4} \int d^2x F_{\mu\nu} F^{\mu\nu}$.

Integrating out the fermionic degrees of freedom, one obtains an effective action for the U_{ij}^μ variables alone

$$S_{\text{eff}}(U) = S_G(U) - \text{Tr} \ln G(U). \quad (2.9)$$

However, as discussed in Ref. 2), one needs a Hermitian operator, bounded below, to simulate the variation of $\text{Tr} \ln G$ by pseudofermionic variables. G does not satisfy this requirement, but G and $\bar{G}$ have the same spectrum determinant. Thus one can use the operator $K = \bar{G}G$ to implement the method of Ref. 2) according to the equation

$$S_{\text{eff}}(U) = S_G(U) - \frac{1}{2} \text{Tr} \ln K(U). \quad (2.10)$$

This greatly corresponds to describing the fermions by a second-order formalism, as done by Feynman and Gell-Mann¹³⁾. The Dirac equation is replaced by the equation

$$\{ -D_\mu D^\mu + g^2 \sigma^{\mu\nu} F_{\mu\nu} + m^2 \} \psi = 0, \quad (2.11)$$

where

$$\sigma^{\mu\nu} = \frac{1}{2} [\gamma^\mu, \gamma^\nu].$$

The form of the lattice operator $K(U)$ is best understood by having in mind the various terms in the right-hand side of Eq. (2.11). Simple algebra

gives the following structure for the quadratic form

$$S_{PF} = (\bar{\varphi}, K(U)\varphi). \quad (2.12)$$

(Here and from now on we denote the pseudofermionic variables, which, as we recall from Ref. 2), are ordinary c numbers, by ϕ_{ij} .) S_{PF} contains a term

$$- \sum_{ij} \{ \bar{\varphi}_{i+2j} U_{i+1j}^* U_{ij}^* \varphi_{ij} - \bar{\varphi}_{ij} \varphi_{ij} \}. \quad (2.13)$$

Together with the analogous terms, where ϕ_{ij} is coupled with $\bar{\phi}_{i-2j}$, $\bar{\phi}_{ij+2}$ and $\bar{\phi}_{ij-2}$ (see Fig. 1a), this term constitutes the lattice version of the covariant Laplacian $-D_\mu D^\mu$. Notice, however, that the step, in the construction of the discrete Laplacian, is by two lattice units rather than by one. This corresponds to the fact that in Eq. (2.11) the components ψ^+ and ψ^- appear decoupled.

S_{PF} contains of course a term

$$\sum_{ij} \mu^2 \bar{\varphi}_{ij} \varphi_{ij} \quad (2.14)$$

and then terms of the form

$$\sum_{ij} i(-1)^{ij} \bar{\varphi}_{i+1j+1} (U_{i+1j}^4 U_{ij}^* - U_{ij+1}^* U_{ij}^4) \varphi_{ij}. \quad (2.15)$$

In this last expression the field ϕ_{ij} is coupled to its nearest neighbour along the diagonal : $\bar{\phi}_{i+1j+1}$. There are two possible transports from site ij to site $i+1j+1$ along opposite sides of the plaquette with diagonals between ij and $i+1j+1$. The difference between the two corresponding transport factors appears in the coupling. But this difference is related, by a phase factor, to $1 - U_{\square ij}$ and thus measures the electromagnetic field strength on the lattice. There are three additional terms of the form (2.15) in S_{PF} , where ϕ_{ij} is similarly coupled to the other neighbours along the diagonals (see Fig. 1b). Altogether these terms reproduce the $\sigma^{\mu\nu} F_{\mu\nu}$ term of Eq. (2.11).

Although assigning different chirality components to different sites reduces the severity of the multiplication of modes, the problem is not entirely solved. Heuristically, we may argue that separating the components of ψ reduces

the number of degrees of freedom by a factor of 2, whereas there are four points in a cell of size $2a$. Thus we expect the fermions to appear doubled. This is best verified by expressing the action in terms of Fourier conjugate variables. We define vectors x^μ of components $x^1 = ia$, $x^2 = ja$ and set

$$\varphi_{ij} = \frac{1}{4\pi} \int_{-\pi/a}^{\pi/a} d^2p \, e^{ip_\mu x^\mu} \hat{\varphi}(p) \quad (2.16)$$

(the explicit dependence on the lattice spacing a and a few other factors have been introduced here to achieve proper normalization to the continuum). Considering for simplicity the free case ($U_{ij}^\mu = 1$), we find

$$S_{PF} = \frac{1}{4a^2} \int_{-\pi/a}^{\pi/a} d^2p \left\{ 2(1 - \cos 2p_1 a) + 2(1 - \cos 2p_2 a) + \mu^2 \right\} \hat{\tilde{\varphi}}(p) \hat{\varphi}(p). \quad (2.17)$$

It is actually convenient to define the Brillouin zone by

$$-\frac{\pi}{2a} \leq p_1, p_2 \leq \frac{3\pi}{2a}.$$

We see then that the inverse propagator

$$K_0^{-1} = \frac{(1 - \cos 2p_1 a)}{2a^2} + \frac{(1 - \cos 2p_2 a)}{2a^2} + \frac{\mu^2}{4a^2} \quad (2.18)$$

has four low-frequency points, i.e., there are four vectors $p_\mu^{(k)}$ ($k = 1 \dots 4$) such that, setting $p_\mu = p_\mu^{(k)} + p'_\mu$, the propagator takes for small p'_μ the continuum form

$$K_0^{-1} \approx (p')^2 + \frac{\mu^2}{4a^2}. \quad (2.19)$$

(Incidentally, this establishes the relation $\mu = 2ma$ between the mass m of the continuum theory and the dimensionless parameter μ .)

The low-frequency points are the origin of momentum space $p_\mu^{(1)} = 0$, and the other three points obtained by translating any component of $p_\mu^{(1)}$ by π/a :

$$p_\mu^{(2)} = \left(\frac{\pi}{a}, 0 \right), \quad p_\mu^{(3)} = \left(0, \frac{\pi}{a} \right), \quad p_\mu^{(4)} = \left(\frac{\pi}{a}, \frac{\pi}{a} \right).$$

Let us define

$$\varphi^{(k)}(p_\mu) = \hat{\varphi}(p_\mu^{(k)} + p_\mu) \quad (2.20)$$

and consider only neighbourhoods of the low-frequency points (i.e., small p_μ in all $\phi^{(k)}$). Since

$$e^{i p_\mu^{(4)} x_\mu} = e^{i \pi (i+j)} = (-1)^{i+j},$$

we see that forming the combinations $\eta_\pm = \phi^{(1)} \pm \phi^{(4)}$ corresponds to selecting even or odd sites, and the same is true of the combinations $\eta'_\pm = \phi^{(2)} \pm \phi^{(3)}$. Thus these linear combinations can be associated, in the continuum limit, to the two chirality components of the Dirac field. However, there are still two independent modes in the theory, η and η' , which in the continuum limit appear to be coupled only through their common interaction with the gauge field. Thus in its present formulation, the lattice action really describes a system of two charged massive fermions coupled to the electromagnetic field.

This doubling is not a welcome feature, since some of the properties of the system under investigation crucially depend on the number of fermion species. To eliminate the doubling in the continuum limit we resort to the following stratagem. A theory, where two identical fermions appear with the same quadratic action $(\bar{\psi}, \Delta(U)\psi)$ and are coupled only to the gauge field, produces, upon integration over the fermionic degrees of freedom, an effective action :

$$\begin{aligned} S_{\text{eff}} &= S_G - 2 \text{Tr} \ln \Delta = \\ &= S_G - \ln (\det \Delta)^2. \end{aligned} \quad (2.21)$$

Assuming that the determinant of the lattice operator G (and correspondingly also $\det K$) undergoes an analogous factorization in the continuum limit, we shall use for effective action

$$\begin{aligned} S_{\text{eff}} &= S_G - \frac{1}{2} \text{Tr} \ln G = \\ &= S_G - \frac{1}{4} \text{Tr} \ln K. \end{aligned} \quad (2.22)$$

On the lattice, this action will produce a violation of fundamental axioms, but we expect the violation to disappear in the continuum limit and then recover the theory with a simple fermion (although some care may be needed for a proper definition of the axial current). Returning to the method of Ref. 2), in practice

the upgrading of the pseudofermionic variables will be done (n times for each updating of the U_{ij}^H) with the action $(\bar{\phi}, K(U)\phi)$; the upgrading of the gauge variables will then be done with the action

$$S_G = \frac{1}{4} \sum_{ij, i'j'} \overline{\phi_{ij}} \phi_{i'j'} K(U)_{ij, i'j'} ,$$

where $\overline{\phi_{ij}} \phi_{i'j'}$ stand for the averages taken over the n pseudofermionic steps.

It is known that the one-flavour massless Schwinger model (in the continuum) undergoes a breaking of chiral symmetry. This can be seen by noticing that 10)

$$\langle \bar{\psi}(x) \psi(x) \bar{\psi}(0) \psi(0) \rangle \xrightarrow{x \rightarrow \infty} C , \quad (2.23)$$

where

$$C = \frac{g^2}{8\pi^3} \exp(2\gamma)$$

and γ is the Euler-Mascheroni constant. This result breaks the cluster decomposition, i.e., the vacuum is not a pure state.

We can decompose the vacuum as an integral over clustering ω vacua, with

$$\langle \bar{\psi} \psi \rangle_{\omega} = A \cos \omega , \quad \langle \bar{\psi} \gamma_5 \psi \rangle_{\omega} = A \sin \omega .$$

If the $m = 0$ theory is approached as the limit of $m \neq 0$ theories, the $\omega = 0$ vacuum is automatically selected :

$$\lim_{m \rightarrow 0} \langle \bar{\psi} \psi \rangle = A . \quad (2.24)$$

It is also evident that

$$C = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\omega A^2 \cos^2 \omega = \frac{1}{2} A^2 \quad (2.25)$$

We finally get

$$A = \sqrt{2C} . \quad (2.26)$$

The relation between the continuum $\langle \bar{\psi} \psi \rangle$ and the lattice expectation value $\langle \bar{\phi} \phi \rangle$ is most easily found by expressing $\langle \bar{\psi} \psi \rangle$ as a logarithmic derivative of the partition function with respect to the continuum mass parameter m . Leaving the further averaging over the gauge field configuration implicit, we have :

$$\begin{aligned} \langle \bar{\psi} \psi \rangle &= \frac{1}{Na^2} \frac{\partial}{\partial m} \ln e^{-S_{\text{eff}}} = \\ &= \frac{1}{Na^2} \frac{\partial}{\partial m} \ln e^{\frac{1}{4} \text{Tr} \ln K} \end{aligned} \quad (2.27)$$

(N denotes the number of points in the lattice). On the other hand,

$$\langle \bar{\phi} \phi \rangle = \frac{1}{N} \frac{\partial}{\partial \mu^2} \ln e^{\text{Tr} \ln K} \quad (2.28)$$

The relation

$$\langle \bar{\psi} \psi \rangle = 2m \langle \bar{\phi} \phi \rangle = \frac{\mu}{a} \langle \bar{\phi} \phi \rangle \quad (2.29)$$

follows immediately. Thus chiral symmetry breaking will manifest itself with a divergence of $\langle \bar{\phi} \phi \rangle$ as $1/\mu$ when $\mu \rightarrow 0$. This pattern of symmetry breaking is rather peculiar to our formulation.

3. - QUENCHED FIELD THEORY : THE STAGGERED CASE

In the free field case, Eq. (2.17) implies the following result for the expectation value $\langle \bar{\phi} \phi \rangle$:

$$\langle \bar{\phi} \phi \rangle = \frac{1}{\pi^2} \int_{-\pi}^{\pi} d^2 p \left\{ 2(1 - \cos 2p_1) + 2(1 - \cos 2p_2) + \mu^2 \right\}^{-1} \quad (3.1)$$

which, in the small μ limit behaves as :

$$\langle \bar{\phi} \phi \rangle = \frac{1}{4\pi} \ln \left(\frac{32}{\mu^2} \right) + O(\mu^2) \quad (3.2)$$

Spontaneous breaking of chiral symmetry, i.e., a non-vanishing limit of $\langle \bar{\psi}\psi \rangle \propto \mu \langle \bar{\phi}\phi \rangle$ for $\mu \rightarrow 0$, requires a more singular behaviour of $\langle \bar{\phi}\phi \rangle$. This can come from the effect of the gauge field on the propagation of fermions.

If we denote by $\langle \bar{\phi}\phi \rangle_U$ the average value of $\bar{\phi}\phi$ (or, in general, the value of any Green's function) in the presence of a definite external gauge field U_{ij}^μ , the quantum mechanical expectation value $\langle \bar{\phi}\phi \rangle$ is obtained by averaging $\langle \bar{\phi}\phi \rangle_U$ over all gauge field configurations, with a measure given by

$$e^{-S_{\text{eff}}} = e^{-S_0 + \frac{1}{4} \text{Tr} \ln K} \quad (3.3)$$

[see Eq. (2.22)]. In the presence of N species of identical fermions (N flavours), the measure factor would be

$$e^{-S_{\text{eff}}} = e^{-S_0 + \frac{N}{4} \text{Tr} \ln K} \quad (3.4)$$

A first approximation to the effect of the gauge field on the fermion observables may be achieved by setting $N = 0$ in Eq. (3.4). This amounts to neglecting the contributions from the fermionic vacuum polarization diagrams and, using a terminology developed in the theory of condensed matter, we shall call the expectation values thus obtained "quenched".

For general values of the gauge coupling parameter β , the problem of deriving quenched averages must still be approached numerically although the computation is simplified, and we shall return to it in the next section. In the extreme case $\beta = -\infty$, however, the normal averages reduce to the quenched ones and both can be evaluated analytically, as we now show.

When $\beta = -\infty$, the only gauge field configurations to contribute are those where all plaquettes have maximal internal energy : $E_{\square} = 1 - \text{Re} U_{\square} = 2$ (fully "frustrated" case). By choosing a suitable gauge, these field configurations can be brought to the form

$$U_{ij}^x = 1 \quad , \quad U_{ij}^y = (-1)^i \quad (3.5)$$

The Wilson loop behaves as $\exp i\pi S$, S being its surface in units of the lattice spacing squared. The gauge chosen has the advantage that the field configuration is explicitly invariant under translations of even numbers of lattice sites. In order to use this symmetry to the maximum, we again introduce the fields $\phi^{(k)}(p)$ of Eq. (2.20) and restrict the Brillouin zone to $-\pi/2 \leq p_1, p_2 \leq \pi/2$ (always with $a = 1$). In Fourier space the action then takes the form

$$S_{PF} = \int_{-\pi/2}^{\pi/2} d^2 p \left\{ [2(1 - \cos 2p_1) + 2(1 - \cos 2p_2) + \mu^2] \sum_i \bar{\varphi}^{(i)} \varphi^{(i)} + 8i \sin p_1 \sin p_2 [\bar{\varphi}^{(1)} \varphi^{(1)} - \bar{\varphi}^{(1)} \varphi^{(2)} + \bar{\varphi}^{(2)} \varphi^{(4)} - \bar{\varphi}^{(4)} \varphi^{(2)}] \right\}. \quad (3.6)$$

From this one easily obtains

$$\sum_i K_{ii}^{-1}(p) = 2 \left[\frac{1}{4(\sin p_1 + \sin p_2)^2 + \mu^2} + \frac{1}{4(\sin p_1 - \sin p_2)^2 + \mu^2} \right], \quad (3.7)$$

where K_{ij}^{-1} denotes the momentum space propagator of the fields $\phi^{(i)}(p)$. In the limit $\mu^2 \rightarrow 0$ the propagator becomes singular on the two lines $p_1 = p_2$ and $p_1 = -p_2$. $\langle \bar{\phi} \phi \rangle$ is given by

$$\langle \bar{\varphi} \varphi \rangle = \frac{1}{4\pi^2} \int_{-\pi/2}^{\pi/2} d^2 p \sum_i K_{ii}^{-1}(p). \quad (3.8)$$

If we set $p_1 = p_2 + q$ in the second term, we obtain, for small q , the following integral

$$\int dp_2 \frac{1}{\cos^2 p_2 \sin^2 q + \mu^2}, \quad (3.9)$$

which gives

$$\langle \bar{\varphi} \varphi \rangle \approx \frac{B}{\mu} \ln \left(\frac{1}{\mu} \right), \quad B \cong 0.44. \quad (3.10)$$

Consequently we find a spontaneous symmetry breaking of the chiral symmetry in the sense that $\langle \bar{\psi}\psi \rangle$ goes like $\ln(1/\mu)$ as $\mu \rightarrow 0$, i.e., it is divergent and not going to zero. The divergence of $\langle \bar{\psi}\psi \rangle$ when $\mu \rightarrow 0$ is a pathology of the $\beta = -\infty$ case and, as we shall see later, disappears for $\beta \neq -\infty$.

The conclusion is that in the limit $\beta \rightarrow -\infty$ chiral symmetry is broken. In the next section we will see that this breaking is also present for finite β in the quenched case. Notice that no analytic solution is available for $\beta = 0$ at arbitrary fermionic mass, contrary to what happens in the Hamiltonian formalism.

4. - QUENCHED FIELD THEORY : THE GENERAL CASE

For general values of β there is no way of analytically evaluating the quenched average of $\bar{\phi}\phi$ and we must resort to numerical computations. We have considered a 16×16 lattice and, by the standard Monte Carlo procedure, have brought the dynamical variables U_{ij}^μ to statistical equilibrium with respect to the measure e^{-S_G} , given by the exponential of the gauge action alone. We have selected $\beta = 3$ as a reasonable intermediate value between the strong coupling domain, where the structure of the lattice would show up too much, and the domain of very weak coupling, where a 16×16 lattice becomes too small to accomodate typical correlation lengths.

The average $\langle \bar{\phi}\phi \rangle$ should first be computed over all points of the lattice and then over several configurations of the external field U . We have assumed that the lattice average already gives a good approximation to the quenched average (indeed, for an infinite lattice, the volume average of $\langle \bar{\phi}\phi \rangle$ is the quenched average) and so have computed $\langle \bar{\phi}\phi \rangle$ in the background provided by the U_{ij}^μ obtained at the end of a very long Monte Carlo simulation (several thousand iterations) of the pure gauge system.

The expectation value $\langle \bar{\phi}\phi \rangle$ can be derived by a Monte Carlo simulation over the pseudofermionic variables ϕ_{ij} , with the action

$$S_{PF} = \sum_{ij, i'j'} \bar{\varphi}_{ij} K(U)_{ij, i'j'} \varphi_{i'j'}, \quad (4.1)$$

[see Eqs. (2.12)-(2.15)], or it can be expressed in terms of the Green's function for the operator K , according to the equation

$$\langle \bar{\psi} \psi \rangle = \frac{1}{N} \sum_{ij} \{K(U)^{-1}\}_{ij,ij} \quad (4.2)$$

($N = 16^2$ = number of points in the lattice). The inverse operator K^{-1} can in turn be determined recursively, by a relaxation procedure, as the limiting value of the sequence defined by the equations

$$\begin{aligned} \{K^{-1}\}_{ij,i'j'}^{(0)} &= 0, \\ \{K^{-1}\}_{ij,i'j'}^{(l+1)} &= \{K^{-1}\}_{ij,i'j'}^{(l)} + \epsilon \left[\delta_{ij,i'j'} - \sum_{i''j''} K_{ij,i''j''} \{K^{-1}\}_{i''j'',i'j'}^{(l)} \right] \end{aligned} \quad (4.3)$$

It is evident that

$$\lim_{l \rightarrow \infty} \{K^{-1}\}^{(l)} = K^{-1} \quad (4.4)$$

if the limit exists. We have found that for $0 < \epsilon < \epsilon_c \approx 0.2$ (ϵ_c is a function of β and μ) the sequence $\{K^{-1}\}^{(l)}$ is convergent, while for $\epsilon > \epsilon_c$ it diverges, oscillating with period 2. In the actual computation we have used a value of ϵ slightly smaller than ϵ_c and iterated the equation until the result appeared to converge with a relative error $< 10^{-3}$. The determination of $\langle \bar{\psi} \psi \rangle$ by the relaxation method requires a longer computer time than if one uses the Monte Carlo algorithm (in particular, one must evaluate $\{K^{-1}\}_{ij,i'j'}^{(l)}$ for all pairs $ij, i'j'$, although only the diagonal values $\{K^{-1}\}_{ij,ij}$ are eventually used); the statistical error inherent in the Monte Carlo method is, however, avoided.

In Fig. 2 we exhibit the result of the computations for values $\mu = 0.1, 0.2, 0.4, 0.6, 0.8, 1$ and 1.2 . From the exact solution of the Schwinger model one expects [see Eqs. (2.23)-(2.26)]

$$\langle \bar{\psi} \psi \rangle = \frac{g}{2\pi\sqrt{\pi}} e^{\gamma} \quad (4.5)$$

for $m = 0$ in the continuum limit. With Eqs. (2.28) and (2.29) this becomes

$$\lim_{\mu \rightarrow 0} \mu \langle \bar{\psi} \psi \rangle = \frac{1}{2\pi \sqrt{\pi\beta}} e^{\gamma}. \quad (4.6)$$

The value of this last expression for $\beta = 3$ is reported on the $\mu = 0$ axis in Fig. 2 (and Fig. 3).

From Fig. 2 one notices that the values obtained for $\langle \bar{\psi} \psi \rangle_{\text{quenched}}$ with the Monte Carlo method and the relaxation method are consistent, and, moreover, that the numbers clearly tend to a non-vanishing limit for $\mu \rightarrow 0$.

The dashed-dotted line in Fig. 2 gives the values of $\mu \langle \bar{\psi} \psi \rangle$ in the free case [Eq. (3.1)]. The solid line gives the result of a quadratic fit to the values of $\mu \langle \bar{\psi} \psi \rangle$ (relaxation method) at $\mu = 0.2, 0.4$ and 0.6 . There is, of course, a certain degree of ambiguity in the extrapolation to $\mu = 0$, made particularly evident by the rapid variation of the free-field results. To take into account this margin of uncertainty we also present the extrapolation obtained from a quadratic fit not to $\mu \langle \bar{\psi} \psi \rangle$ directly, but to the difference $\mu \langle \bar{\psi} \psi \rangle - \mu \langle \bar{\psi} \psi \rangle_{\text{free}}$ (dashed line).

In principle, the ambiguity in the extrapolation could be resolved by going to smaller values of μ , but there is then a conflict with the finite size of the lattice. We have already seen how crucially a non-zero expectation value of $\langle \bar{\psi} \psi \rangle$ for $\mu = 0$ depends on the low frequency part of the fermion propagation. A lattice of $L \times L$ sites introduces a discretization of the momenta, with a gap of the order $\Delta p \approx 2\pi/L$ (or even $4\pi/L$ if the unit cell indeed contains four sites). Thus one would expect finite size distortions when μ becomes comparable with Δp . In the free case for instance, with periodic boundary conditions, the single zero-mode at the origin produces a divergent result $\mu \langle \bar{\psi} \psi \rangle_{\text{free}} \sim 1/N\mu$ ($N = L^2 =$ number of points in the lattice), rather than the expected $\mu \ln \mu$. But using antiperiodic boundary conditions instead, the modes are displaced and $\mu \langle \bar{\psi} \psi \rangle_{\text{free}}$ goes to zero linearly in μ without any $\ln \mu$ factor. We expect the randomness introduced by the gauge field, with its averaging effect, to solve a little the problems associated with the finite size ; but in any case we have estimated $\mu = 0.2$ to be the lowest reliable value with a 16^2 lattice. We have nevertheless performed computations at $\mu = 0.1$, but prefer to attribute them only indicative value.

Returning to the results displayed in Fig. 2, the computation at $\mu = 0.1$ seems to favour the fit on the unsubtracted values (solid line). Both fits though lead to a non-vanishing value of $\langle \bar{\psi}\psi \rangle$ for $\mu = 0$ and to spontaneous breaking of chiral symmetry. If anything, the quenched computation seems to produce too large a value of $\langle \bar{\psi}\psi \rangle_{\mu=0}$: as we shall see in Section 6, this effect can be attributed to the lack of dynamical feedback from the fermions onto the gauge field.

5. - THE MONTE CARLO METHOD : 2x2 LATTICE

The goal of the Monte Carlo simulation is to generate U_{ij}^μ fields with probability distribution proportional to

$$\exp \{ - S_{\text{eff}} \} = \exp \{ - S_G + \frac{1}{4} \text{Tr} \ln K \}.$$

Once this is achieved, the computation of correlation functions of fermions is not a serious problem. The basic idea of Ref. 2 is that, although computing the exact variation of $S_G - \frac{1}{4} \text{Tr} \ln K$ in an upgrade $U_{ij}^\mu \rightarrow U_{ij}^\mu + \delta U_{ij}^\mu$ is too time consuming, for small δU_{ij}^μ the variation of S_{eff} can be linearized

$$\delta S_{\text{eff}} = \delta S_G - \frac{1}{4} \text{Tr} K^{-1} \delta K \quad (5.1)$$

and the simulation may proceed rapidly if a fast algorithm for the computation of the Green's function is available ^{*)}. In Ref. 2) it was further proposed that sufficiently approximate values for K^{-1} could be evaluated by a Monte Carlo simulation over a parallel system of pseudofermionic, c number variables ϕ_{ij} . n upgrading steps are done for these variables with action $S_{\text{PF}} = (\bar{\phi}, K(U)\phi)$ and the Green's functions are approximated by

$$\{ K(U)^{-1} \}_{ij, i'j'} \cong \overline{\bar{\phi}_{ij} \phi_{i'j'}} \equiv \frac{1}{n} \sum_k \bar{\phi}_{ij}^{(k)} \phi_{i'j'}^{(k)}, \quad (5.2)$$

^{*)} Although some systems (think for instance of the Ising model) do not allow small steps in the upgrading, δU_{ij}^μ can always be taken small if the range of the dynamical variables is continuous ; moreover, one expects the small fluctuations to become the relevant ones when one approaches the continuum limit.

where $\phi_{ij}^{(k)}$ denotes the values met in the n pseudofermionic steps. The approximate Green's functions are then used to upgrade once all the U_{ij}^μ . Exact results are obtained when $n \rightarrow \infty$ and the error is expected to become proportional to $1/n$. The value of n necessary to get good results changes from system to system and, as is usually the case with Monte Carlo simulations, the validity of the approximation must be estimated from the stability of the results. Generally speaking, one expects faster convergence if the correlation lengths are not too large.

In our simulation the gauge variables U_{ij}^μ have been upgraded by adding to their phase a random angle θ , with a distribution symmetric centered around the origin, and a normal deviation $\Delta\theta \approx 0.2$. The pseudofermionic variables have been upgraded by adding to their real and imaginary parts independent random variables, $r_{R,I}$, again with a distribution symmetric centered around the origin and a deviation $\Delta r \approx 0.2$.

On a very small lattice, extending for only two sites in the two directions, the determinant of the 4×4 matrix $K_{ij,i'j'}(U)$ is simple enough to be computed and used in a Monte Carlo simulation. One can then upgrade the δU_{ij}^μ variables either by following our method or with a direct Monte Carlo simulation with a measure factor incorporating $\det K$.

To check the validity of the method we have carried out Monte Carlo computations for the 2×2 system either by working with the gauge variables alone, and with measure factors $(\det K)e^{-S_G}$ (fermionic case) and $(\det K)^{-1}e^{-S_G}$ (bosonic case), or by using the coupled system of gauge and pseudofermionic variables. We have also considered the case where the determinant appears at the denominator to see the relevance of the dynamical feedback from the pseudofermions. In the bosonic case, of course, the computation reduces to the ordinary Monte Carlo simulation of a gauge field coupled to a bosonic matter field and the evolution equations guarantee the exactness of the results with $n = 1$. (In these checks we have not used the "demultiplication" trick of taking the fourth root of the determinant ; correspondingly $S_{\text{eff}} = S_G \pm \text{Tr} \ln K$).

The results for $\langle \bar{\phi}\phi \rangle$ are reproduced in the Table and are rather satisfactory, even for low values of n . (50,000 Monte Carlo iterations have been used to reach good statistical accuracy ; on larger lattices the volume factor produces comparable accuracy with a lot less iterations.) The mean value of $\bar{\phi}\phi$ decreases drastically when going from the bosonic system to the fermionic one. Indeed, the

fermionic determinant at numerator decreases the probability of encountering those gauge field configurations leading to small eigenvalues of K and to large $\text{Tr } K^{-1}$. Conversely these configurations are enhanced in the bosonic case.

β	μ	Fermionic/ Bosonic System	Direct	New Algorithm	n
3	1	F	0.158 ± 0.002	0.156 ± 0.004	5
3	1	B	0.677 ± 0.007	0.667 ± 0.005	5
0.2	0.4	F	0.267 ± 0.003	0.285 ± 0.006	5
0.2	0.4	B	3.10 ± 0.03	3.10 ± 0.4	1

Numbers determined for the expectation value $\langle \bar{\phi}\phi \rangle$ on a small (2x2) lattice either with a direct Monte Carlo simulation of the gauge system with the appropriate effective action or using the algorithm of Ref. 2).

6. - MONTE CARLO SIMULATIONS : 16x16 LATTICE

We have performed simulations for the coupled system of gauge variables and pseudofermionic variables on a 16x16 lattice at $\beta = 3$. We started from the equilibrium configuration of the pure gauge system, already used in the quenched simulations, and vanishing pseudofermionic fields. 1000 iterations, with $n = 5$ (hence altogether 1000 Monte Carlo steps per U_{ij}^μ , 5000 Monte Carlo steps per ϕ_{ij}) were made keeping the mass parameter fixed at $\mu = 1.2$. The final configuration of the U and ϕ variables was recorded on magnetic tape and used as the initial configuration for a run of 1000 iterations at $\mu = 1$. The final configuration was again used as the initial configuration for a run at $\mu = 0.8$ and, repeating the procedure, runs of 1000 iterations, all with $n = 5$, were made at progressively lower values $\mu = 0.6, 0.4, 0.2$ and 0.1 . The final configurations from the simulations at $\mu = 0.6 \div 0.1$ were also used as initial configurations for runs at the same values of the mass, but $n = 10$. The final configurations of these simulations were used as starting ones for runs with $n = 30$ and in the same way simulations with $n = 60$ and, for $\mu = 0.1$, $n = 120$ were also made. With the highest values of n smaller numbers of bosonic iterations (from a few hundred down to one hundred for $n = 120$) were used to evaluate the averages.

The details of the upgrading procedure are the same as those described in Section 5. With a reasonably optimized programme, the CP time requirement on a CDC 7600 was contained within an acceptable $(25+15 n)$ milliseconds per iteration.

The results for $\mu\langle\bar{\phi}\phi\rangle$ are presented in Fig. 3 (where the free-field values, given by the dashed-dotted line, are also reproduced). Comparing the quenched values (Fig. 2) with the values obtained with the full simulation, one immediately notices that the inclusion of the feedback from the fermions tends to lower the expectation value of $\bar{\psi}\psi$. This is in agreement with what one expects from the rôle played by the fermionic determinant (cf. the discussion at the end of the previous section) and is a welcome modification, since in the $\mu \rightarrow 0$ limit the quenched values appeared too high. With a small number ($n = 5, 10$) of pseudofermionic steps, however, the algorithm seems to over-correct, in particular for smaller values of the mass ($\mu = 0.1$ and 0.2) where $\mu\langle\bar{\phi}\phi\rangle$ comes out, with $n = 5$ or 10 , as low as the free value. Higher numbers of pseudofermionic iterations are apparently needed in order to find an acceptable approximation to the Green's functions. However, one notices a certain degree of stability of the results with $n = 30$ and 60 all the way down to $\mu = 0.2$. Only for $\mu = 0.1$ is the increase in $\mu\langle\bar{\phi}\phi\rangle$ going from $n = 30$ to $n = 60$ marked and a further increase is observed passing to 120 pseudofermionic steps. Clearly a critical slowing down of convergence is occurring as $\mu \rightarrow 0$.

As we have discussed already (cf. Section 4), too low values of μ are in any case unreliable because of finite size effects. Thus we have extrapolated to $\mu = 0$ using the results (with highest n) at $\mu = 0.2, 0.4$ and 0.6 . The solid line in Fig. 3 represents a quadratic fit through the points and the dashed line an interpolation obtained by quadratically fitting not $\mu\langle\bar{\phi}\phi\rangle$ directly, but $\mu\langle\bar{\phi}\phi\rangle - \mu\langle\bar{\phi}\phi\rangle_{\text{free}}$. This last fit is presented for fairness, to remind us that the extrapolation to $\mu = 0$ is by no means unambiguous. The results at $\mu = 0.1$, however, seem to support the validity of the former (direct) fit. For $\mu = 0$ this gives $\langle\bar{\psi}\psi\rangle \approx 0.077$, which is in reasonably good agreement with the Schwinger model value $\langle\bar{\psi}\psi\rangle \approx 0.092$.

7. - CONCLUSIONS

In this article we have shown that the "defermionization" procedure proposed in Ref. 2) can be efficiently used to study fermionic systems with a high number of degrees of freedom. Other, somehow related, methods have recently been presented in the literature¹⁴⁾⁻¹⁶⁾. The basic ideas of integrating out the fermionic degrees of freedom and of evaluating the ratio of the determinants by means of Green's functions are maintained : the alternative proposals differ, however, from Ref. 2) in the technique used to compute the Green's functions themselves. The relaxation method of Ref. 14) seems to require definitely too long CP times. More promising appears the suggestion of Refs. 15) and 16) of upgrading the Green's function, once calculated, by a linearized formula. All these methods, however, imply an increase of CP time by factors at least proportional to the number of degrees of freedom (rather than the fixed number of pseudofermionic steps). Moreover, all the Green's functions must be computed and stored and the memory requirements become soon unmanageable as the size of the system increases. For smaller systems, however, the results are satisfactory.

Maybe some combination of our method and these alternative proposals will lead, even for larger systems, to faster and more accurate results, than can be achieved with our technique alone. At present, however, our method has allowed a numerical verification of the spontaneous breaking of chiral symmetry, with a value of $\langle \bar{\psi}\psi \rangle$ consistent with the exact results for the continuum theory.

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FIGURE CAPTIONS

Fig. 1 a), b) Diagrammatic representation of the terms in the operator K .

Fig. 2 Results for the quenched expectation value $\langle \bar{\psi}\psi \rangle$:
x points obtained with the relaxation method ;
• points obtained with a Monte Carlo simulation ;
* theoretical value in the Schwinger model.
The lines represent :
—— quadratic fit through the points at $m = 0.2, 0.4, 0.6$;
--- quadratic fit to $\langle \bar{\psi}\psi \rangle - \langle \bar{\psi}\psi \rangle_{\text{free}}$ at the same values of m ;
---- expectation value in the free theory.

Fig. 3 Results for $\langle \bar{\psi}\psi \rangle$ obtained with the method of Ref. 2), and with 5 (•), 10 (o), 30 (■), 60 (x) and 120 (▲) pseudofermionic steps per bosonic iteration (the marks are offset to avoid overlap). The legend for * and the lines is the same as in Fig. 2.

FIG. 1a

FIG. 1b

FIG.2

FIG.3