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SOME APPLICATIONS OF A NEW STOCHASTIC METHOD IN LATTICE THEORIES*

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ABSTRACT

Some applications of a new stochastic method to the numerical study of lattice models is presented. The method is directly applicable to lattice path integrals in the presence of fermionic degrees of freedom. It is also relevant for the evaluation of the partition function of lattice spin systems. We shall describe here the method briefly and present some recent results. The numerical study of Quantum Chromodynamics in the presence of fermionic vacuum polarization and the calculation of the largest eigenvalue of the transfer matrix in the three-dimensional Ising model are the most important applications.

1. INTRODUCTION

It is perhaps the most outstanding problem today in the numerical study of Quantum Chromodynamics to find an efficient method for treating the fermionic degrees of freedom. The problem is twofold there.

One has to treat correctly the kinetic motion of quarks in the presence of their interactions through the non-perturbative gauge field configurations.

In this so-called quenched approximation some preliminary results have been published recently[1], with detailed studies of the hadron spectrum and chiral symmetry breaking.

The other important problem in the numerical study of QCD is to get some estimate about the importance of the fermionic vacuum polarization on the hadron structure, chiral symmetry breaking and the bulk properties of hot and/or dense quark-gluon matter. Practically nothing is known about that.

Here we would like to study a new stochastic method for the full treatment of the fermionic vacuum polarization problem. The method is also a useful tool in the quenched approximation. The essential point is that we give up the notion of exact summation over the propagation of quark orbits inside hadrons, or in vacuum polarization fluctuations. Instead, we wish to evaluate the contribution of quark orbits to the functional integral over the Grassman variables by a stochastic method[2] wich is based on some early work of Neumann and Ulam.

The method is very efficient for the stochastic evaluation of matrix operations over matrices of enormous size whose numerical processing would be impossible otherwise. Therefore, we believe that the method may be relevant not only in quantum field theoretic models but also in condensed matter physics and nuclear physics.

This report is organized in the following way. First we shall give a very brief introduction to the subject and describe some of the mathematical aspects of the method. Next, we shall present a simple test model wich was already briefly described elsewhere[2]. For illustration of applications in condensed matter physics, the largest eigenvalue of the transfer matrix of

the 3-dimensional Ising model is calculated. The related thermodynamical properties of the model are also briefly described[3]. Our next excercise is the detailed study of Dirac's free fermion theory in its second quantized version. For demonstration, we shall calculate there the bulk thermodynamical properties of a relativistic free fermion gas. Finally, we shall present some results in QCD in the presence of quark vacuum polarization. We will mainly concentrate on some bulk thermodynamical properties of the hot quark-gluon plasma.

2. *THE FUNCTIONAL INTEGRAL*

For a general presentation, we will consider now the Euclidean action

$$S=S_0(U)+\Sigma\bar{\psi}_i M_{ij}(U)\psi_j. \qquad (1)$$

in four dimensions. It describes the interaction of a boson field U_i with a fermion field Ψ_i, and the subscripts on the fields refer to the lattice points. Spin and internal symmetry indices are supressed, for simplicity. The matrix $M_{ij}(U)$ designates both kinetic and mass terms for the fermion field, and couplings to the boson field. $S_0(U)$ describes the pure bosonic part of the Euclidean action.

It is important to note that most of the interesting models in quantum field theory, condensed matter physics, and nuclear physics can be brought to a bilinear form in the fermion fields.

The fermion Green's functions can be calculated by inserting sources into the path integral

$$Z(\bar{\eta},\eta) = \int D\bar{\psi}D\psi DU \exp[S+\Sigma_i(\bar{\eta}_i \psi_i+\bar{\psi}_i\eta_i)]. \qquad (2)$$

We will follow here the standard strategy and work directly with a new effective action of the boson fields when the fermionic degrees of freedom are integrated out. Though the effective action becomes non-local in the presence of the fermion determinant, the new procedure maintains the efficiency of the standard Monte Carlo technique where the update time on a site is independent of the lattice volume. The method is applicable in any number of dimensions.

Recently, the fermion problem was solved by Hirsch, Scalapino, Sugar and Blankenbeckler[4] in one space and one time dimension. They follow the evolution of fermion world lines along the Euclidean time direction with an update time independent of the lattice volume. The method is fast and efficient in applications. The generalization of this ingenious idea to higher dimensions remains unsolved but very desirable.

In Quantum Chromodynamics interesting progress has been made[5] using the hopping parameter expansion in Wilson's lattice formulation of fermions[6] and Pade extrapolation in the expansion. Further work is in progress in that direction[7].

We will also use Wilson's lattice fermions in our QCD application but we differ from others in our numerical treatment of the summation over quark paths in the functional integral. For an introduction to the whole subject matter of

fermions and for the discussion of current work of others in the field we have to refer you to some recent review[8].

3. FERMION GREEN'S FUNCTIONS

By taking the functional derivates in Eq.(2) and integrating out the Grassman variables, the fermion correlation function can be written as

$$\langle\bar{\psi}_i\psi_j\rangle = \delta^2/\delta\eta_i\delta\bar{\eta}_j \ln Z\,(\bar{\eta},\eta)_{\bar{\eta}=\eta=0} =$$

$$= 1/Z \int DU\, M_{ij}^{-1}(U)\exp[S_{eff}(U)]\ , \qquad (3)$$

where Z is the partition function (normalization integral) of the boson-fermion system.

The effective action is given by

$$\exp[S_{eff}(U)] = \det[M(U)]\exp[S_0(U)]\ . \qquad (4)$$

and we assume, for simplicity only, that the fermion determinant has positive sign. It is certainly true in QCD with Wilson fermions.

We apply now the Metropolis Monte Carlo method to the evaluation of the functional integral in Eq.(3). Other Euclidean Green functions can be treated similarly.

It was shown by Scalapino and Sugar[10], and by Fucito et al.[11] that a local change U→U=δU implies

$$\exp[S_{eff}(U+\delta U)-S_{eff}(U)] = \det[1+M^{-1}(U)\delta M(U)]\cdot \exp[S_0(U+\delta U)-S_0(U)]. \quad (5)$$

With local boson-fermion coupling the non-trivial change δM in the fermion matrix is restricted to the neighborhood of the updated lattice site. Consequently, we need only a few inverse elements of the large matrix M in each Metropolis step.

At that point we depart from standard procedures. Since the results of a Monte Carlo calculation are always subject to some statistical inaccuracy, it is reasonable to evaluate the decision-making step stochastically. The error analysis becomes subtle but we are not concerned with it here.

4. *THE NEUMANN-ULAM METHOD*

We will calculate the inverse matrix elements of M by some modification of a stochastic method which was first suggested by J. von Neumann and S.M. Ulam, but never published by them[9]. It is a very efficient method for the approximate summation of the Neumann series defined by the inverse of an operator M. Somehow this brilliant idea and its potential use escaped the attention of the particle physics community. We present here a very brief description of the mathematical method.

Assume that the inverse of a matrix M of order m is desired and let H=I-M, where I is the unit matrix. For the method to be applicable, it is necessary and sufficient that the eigenvalues of the matrix $H_{ij}=|H_{ij}|$ are less than one in absolute value.

Note that the above condition can always be arranged by proper normalization. The matrix elements $(M^{-1})_{ij}$ are given by the solutions of the linear system of equations Mx=b , with unit driving vectors on the right-hand side. This equation is equivalent to $(2/\mu)M^{+}Mx=(2/\mu)M^{+}b$ where μ is the first norm of the matrix $M^{+}M$. The driving vector $(2/\mu)M^{+}$ may be decomposed into a linear combination of unit vectors and, with the replacement $M\to(2/\mu)\,M^{+}M$, the method applies even in the worst case.

We decompose the matrix element H_{ik} into $H_{ik}=P_{ik}\cdot R_{ik}$ with the restriction that $P_{ik}>0$ and $\Sigma_r P_{ir}<1$ for all values of i. Consider a random walk on the domain of integers 1,2,...,m. The walk begins at some selected point i and proceeds from point to point with the transition probabilities P_{ik}. The walks stop after k steps at some point s_k with the stop probability $P_{s_k}=1-\Sigma_r P_{s_k r}$.

When the walk stops, a score S_{ij} is registered for the elements in the i^{th} row of the inverse matrix. It is defined by the product of the residues $R_{s_r s_{r+1}}$ along the trajectory $i\to s_1\to s_2\to\ldots\to s_k=j$ divided by the stop probability P_j.

$$S_{ij} = \begin{cases} 0 & \text{if } s_k\neq j \\ R_{is_1}R_{s_1s_2}\ldots R_{s_{k-1}j}P_j^{-1} & \text{if } s_k=j \end{cases} \quad (6)$$

We will prove that the expectation value of the random variable S_{ij} is $(M^{-1})_{ij}$. Indeed, the probability of a walk to follow some trajectory $i \to j$ and to stop at j is $P(i \to j) \cdot P_j = P_i s_1 P_{s_1 s_2} .. P_{s_{k-1} j}$. The expected score is given by the sum over all trajectories from i to j :

$$\langle S_{ij} \rangle = \Sigma P(i \to j) P_j S_{ij} = \Sigma P(i \to j) R(i \to j) \qquad (7)$$

where $R(i \to j)$ is the product of the residues along the trajectory. Since $P_{ij} \cdot R_{ij} = H_{ij}$, Eq.(7) is recognized as the Neumann series expansion for $M^{-1} = (1-H)^{-1}$. The term δ_{ij} in the Neumann series is generated by walks which stop immediately.

It is easy to prove that the variance σ^2_{ij} of the random variable S_{ij} is given by

$$\sigma_{ij}^2 = (Q^{-1})_{ij} P_j^{-1} - (M^{-1})_{ij}^2 \qquad (8)$$

where $Q = (I-K)^{-1}$ with $K_{ij} = H_{ij} \cdot R_{ij}$. The variance of S_{ij} is finite, provided the Neumann series for $Q = (I-K)^{-1}$ exists.

The statistical error on $(M^{-1})_{ij}$ is given by $\sigma_{ij}/\sqrt{N}$ for N walks which all begin at point i. For a given statistical accuracy in the decision-making step of the Metropolis procedure, the required number of walks does not depend on the size of the matrix explicitly. Some implicite size dependence may appear in the calculations through the inverse matrix elements of the operators M and Q in the expression for the variance. The update time in this stochastic procedure is practically independent of the lattice volume.

We will modify now the Neumann-Ulam algorithm for better efficiency in fermionic Monte Carlo procedures[2]. It is not difficult to realize that during a walk which started at point i , one can register the product of residues at each pass through the point j . We define a new random variable S_{ij} as the sum of the products of residues, adding a new term to the score at each pass through the point j . The essential point is that the stop probabilities are eliminated now from the scoring procedure and also from the new random variable S_{ij} , but they still govern the average length of the random walks.

This modification will significantly reduce the stochastic error of the method, since the variance was inversely proportional to the stop probabilities in the original Neumann-Ulam proposal. For random walks with large average length the variance became large in their original suggestion. This problem is eliminated now.

It is straightforward to show that $\langle S_{ij} \rangle = \langle S_{ij} \rangle$ when the stop probabilities P_j are positive. We have also proved that the expectation value $\langle S_{ij} \rangle$ is equal to $(M^{-1})_{ij}$ when the stop probabilities P_j vanish. The original method does not apply in this case.

In order to compare efficiencies, we choose a simple case for illustration when all $R_{ij} = 1$ and the P_j's are all positive. A necessary and sufficient condition for the variance of the random variable S_{ij} to be smaller than σ^2_{ij} is $P_j < e_j/(2-e_j)$, where e_j designates the escape probability from the point j . In practice, this, or some similar condition, always appears and the modified method becomes more efficient.

In the special case when all stop probabilities vanish, one has to stop by fiat. Some bias is introduced then, since the Neumann series becomes trun-

cated after a finite number of terms. This bias is usually not serious in physical applications because it is rare that one has to sample arbitrarily large terms from the expansion.

5. *A SIMPLE TEST MODEL*

This stochastic fermion method was tested first[2] on a four-dimensional boson-fermion model which was suggested by Scalapino and Sugar[10]. The fermion matrix M in Eq.(1) is specified now as

$$M_{ij} = -\Delta_{ij} + (m^2 + gU_i^2)\delta_{ij} \qquad (9)$$

where U_i and ψ_i are a scalar boson field and a spinless fermion field, respectively. Δ_{ij} defines the Laplacian operator on the lattice, m is the bare fermion mass in lattice spacing units, and g designates the dimensional boson-fermion coupling constant.

The functional integral is calculable anatically in this model, and one finds

$$D(i-j) = \langle \bar{\psi}_i \psi_j \rangle = (-\Delta + m^2 + g/2)^{-1}_{ij} \qquad (10)$$

The fermion-boson interaction generates a mass term dynamically, and the renormalized fermion mass is given by $m_r = (m^2 + g/2)^{1/2}$.

In the Neumann expansion of the inverse of the operator M in Eq.(9) the diagonal part D was factored out and the random walks were applied to operator $D^{-1} \cdot M$. This factorization guaranteed the convergence of the expansion.

In the random walks on the 4-dimensional lattice an equal probability of 1/8 was chosen in the eight different directions. Importance sampling was not implemented in the Markov chain of the stochastic process, since the method turned out to be sufficiently fast even in its simplest form.

An illustration of importance sampling in the Neumann-Ulam method will be presented in the next section. The transfer matrix of the 3-dimensional Ising model will be processed this way.

Some results of our calculations are presented in Fig. 1. The complete fermion mass was generated dynamically with the choice m=0. The agreement of the numerical points with the exact analytic form is very satisfactory (the statistical errors are practically not visible on the logarithmic plot). The quenched approximation, where one neglects the fermionic vacuum polarization effects of the fermion determinant in an effective action, is also presented in Fig.1. The contribution of the fermion loops is clearly seen and accurately calculated: $m_q^2/m_r^2 = 0.78$.

The figure caption on the next page gives some information on the parameters of the test model which were used in generating the fermion correlation functions. Test runs for smaller values of the dressed mass of the fermion where longer walks were needed are also available.

The speed and efficiency of the stochastic method is very promising. It took only about 3 hours on a VAX 11/780 to calculate the complete fermion propagator on the $8^3 \cdot 16$ lattice, with relative errors which were only a few percent even for a separation of eight links along the fourth direction.

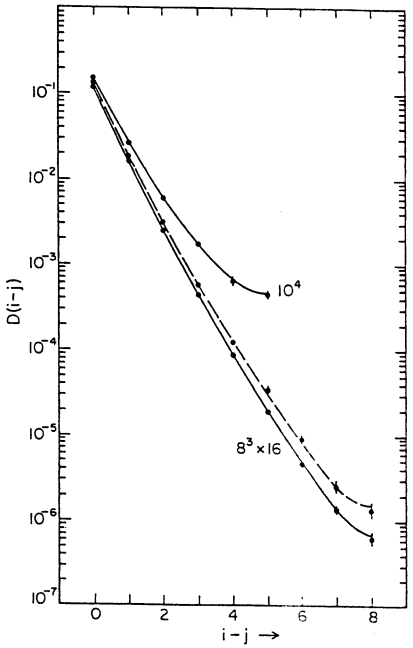

FIG.1. Some numerical results on the fermion correlation function are compared with exact calculations. D(i-j) is depicted for a lattice of $8^3 \cdot 16$ sites with periodic boundary condition and coupling constant $g=2.6a^{-2}$ (in the actual calculations the lattice spacing a was set to unity). The free fermion propagator, with renormalized mass $m_r^2=1.3a^{-2}$ on the same lattice size, is represented by solid line. Results are also presented for a lattice of 10^4 sites with $m_r^2=0.25a^{-2}$. The dashed line is the fit of a free fermion propagator of mass $m_q^2=1.02a^{-2}$ to the results of the quenched approximation on the $8^3 \cdot 16$ periodic lattice with $g=2.6a^{-2}$ and m=0. The continuous curves for the exact propagators are drawn to guide the eye.

6. *THE TRANSFER MATRIX OF THE ISING MODEL*

In this section we would like to discuss an interesting application of our stochasic method to lattice spin systems. This work was done in collaboration with P. Rujan[3]. The results are still rather preliminary but they are very interesting and encouraging for further applications. We note here that the application of a random walk method to the 3-dimensional Ising model, which is also the subject of our discussion here, was also known in the past to some other workers[12].

The partition function of the 3-dimensional Ising model is defined in the usual way

$$Z = \Sigma_{\text{all conf.}} \exp[K \cdot \Sigma_{ij} S_i S_j + H \cdot \Sigma_j S_j] \qquad (11)$$

In Eq.(11) the strength of the spin-spin interaction term includes the inverse temperature and the Boltzmann factor in the standard fashion: $K = J\beta$. The summation in the exponent includes all nearest neighbour interactions.

The summation in front of the exponential is taken over all spin configurations of the 3-dimensional system. A properly normalized external field H is also applied in Eq.(11).

The free energy of the system can be obtained from the partition function Z by

$$F = - k_B T \ln Z/N \ . \qquad (12)$$

It is known that the partition function of the three-dimensional Ising model can be formulated in terms of the largest eigenvalue of the so-called transfer matrix[13].

We want to discuss now this connection. If the size of the lattice is N = lxmxn , the partition function can be written as

$$Z = Tr(V^n) \ , \qquad (13)$$

where the transfer matrix V acts on the spin states of the 2-dimensional layer of lxm sites. This slice has 2^{lxm} spin states.

The transfer matrix can be pictured as an operator which governs the evolution of spin states from slice to slice. Since the vector space of spin states in the 2-dimensional layer is of 2^{lxm} -dimensional, the size of the matrix V is $2^{lxm} \cdot 2^{lxm}$.

It can be shown that in the limit $n \to \infty$ the partition function is dominated by the largest eigenvalue Λ of the matrix V :

$$\lim_{n\to\infty}(\ln Z/n) = \ln\Lambda \ . \qquad (14)$$

We learn from that relation that the properties of the 3-dimensional Ising model of size lxmx∞ can be calculated from the largest eigenvalue of the transfer matrix.

We want to apply now our stochastic method to the calculation of the largest eigenvalue. The matrix V can be decomposed into the product $V = V_1 V_2 V_3$ where

$$V_1 = \Pi(e^{K+\sigma^x_i} e^{-K}),$$

$$V_2 = \Pi\exp(K\sigma^z_i \sigma^z_{i+1}),$$

$$V_3 = \Pi\exp(H\sigma^z_i). \qquad (15)$$

Here σ^x is the Pauli spin-flip operator and σ^z designates the third component of the spin operator.

The term $V_2 V_3$ is identified as the diagonal part of the transfer matrix, since it acts within a given slice of the lattice. V_1 is responsible for the transitions between neighboring 2-dimensional slices.

We organized our random walks according to certain importance sampling as suggested by the structure of the transfer matrix. The transition from a given state of a 2-dimensional spin layer to the next one was governed by V_1 but the walks were weighted by the diagonal part $V_2 V_3$. Some technical details of the random walks will be published elsewhere[3].

We have calculated the largest eigenvalue for lattices of mxmx∞ dimension and various values of m . We were moving about one thousand points in the vector space of spin states and the length of the random walks was also of the order of a few hundred. We obtained five to six digit accuracy in the value of the free energy per spin

$$F = - k_B T/(mxm) \cdot \ln\Lambda .$$

The values of $-F/k_B T$ are depicted in Fig.2 for various lattice sizes.

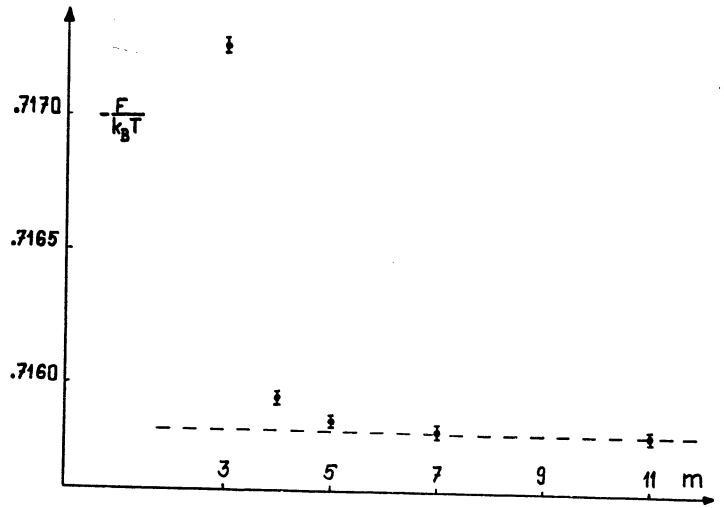

FIG.2. Some numerical results on the free energy per spin in the 3-d Ising model are presented here for various lattice sizes at a fixed value of K . The results are so accurate that surface diagrams from the high-temperature expansion can be seen for m = 3, 4, 5 . The dashed line shows the asymptotic

value of the free energy on the infinite lattice. The accuracy in $-F/k_B T$ is about five decimal places.

The temperature dependence of the free energy is shown if Fig.3 for fixed lattice size. The size m = 11 was chosen to compare our calculations with the results of Ref.12.

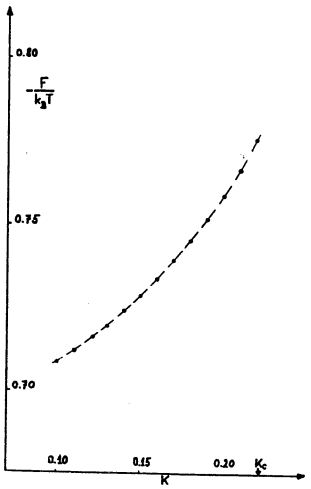

FIG.3. The temperature dependence of the free energy per spin is shown for a lattice of 11x11x∞ dimension. The size of the corresponding transfer matrix is $2^{121} \cdot 2^{121}$. The results agree accurately with the point of Ref.12 at $K = K_c/1.83$. K_c is the critical point of the 3-d Ising model.

The internal energy can be calculated from the known thermodynamical relation

$$U = \delta(-F/K_B T)/\delta K$$

The spin-spin coupling J is set to one here. Simple numerical differentiation gives satisfactory results. The accuracy is greatly increased by correlated sampling of the random walks[13]. Some results are shown in Fig.4.

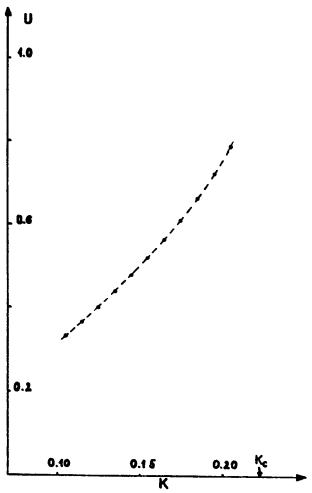

FIG.4. The internal energy U as a function of K for a lattice of 11x11x∞ dimension. The results were obtained by numerical differentiation. The dashed curve is the result of the high temperature expansion on the infinite lattice.

It is very interesting to note that the method gives accurate and direct information about the partition function and the free energy of the system. This direct information is not available in the standard Metropolis Monte Carlo procedure.

7. *QCD AND QUARK VACUUM POLARIZATION*

Following our discussion of fermionic lattice theories in section 2, the functional integral of QCD for the partition function is given by Eqs.(1) and (2). For simplicity, we will consider the SU(2) color gauge group and only one flavor for the quarks. Quarks as Grassman fields live on lattice sites whereas the U matrices of color SU(2) are associated with links in the standard fashion.

We will follow here Wilson's lattice formulation for fermions and the gauge fields[6]. We note here that Larry McLerran and Ben Svetitsky and also Tom DeGrand are also working on the QCD application using second order fermions[14]. We are also investigating the second order formulation and some day we may unite for a joint attack when we get within the radius of three thousand miles. This is about one unit of correlation length.

The fermion matrix M can be written as

$$M = 1 - \kappa \cdot W$$

where κ is the hopping parameter and

$$W_{nm} = (1+\gamma^{\mu}) \cdot U_{n\mu} \cdot \delta_{n,m-\mu} + (1-\gamma^{\mu}) \cdot U^{+}_{n-\mu} \cdot \delta_{n,m+\mu} \qquad (16)$$

The Euclidean Dirac matrices and the color SU(2) matrices connect neighboring lattice sites proportional to the hopping parameter.

Integration over the Grassman variables yields standard formulae

$$\int D\bar{\psi} D\psi \exp[\bar{\psi} M \psi] = \det M,$$

$$\int D\bar{\psi} D\psi \bar{\psi}_i \psi_j \exp[\psi M \psi] = \det M \cdot M^{-1}_{ij}. \qquad (17)$$

The effective fermionic action $S_{eff}(U)$ was defined in section 2 as

$$\exp[S_{eff}(U)] = \det(1-\kappa W). \qquad (18)$$

The only other quantity we have to know for the calculation of composite fermionic operators, like the current correlation function, is the quark propagator M^{-1}_{ij}.

We will apply now our stochastic method to the hopping parameter expansion of the two relevant quantities

$$S_{eff}(U) = -\mathrm{Tr} \Sigma_n (\kappa^{2n}/2n) \cdot W(U)^{2n}, \qquad (19)$$

and

$$M^{-1}(U) = \Sigma_n \kappa^{2n} W(U)^{2n}. \qquad (20)$$

In our calculation of S_{eff} and M^{-1} in Eqs.(19) and (20) we implemented the random walk procedure as it was discussed in section 4. For a first test of the fermionic theory we applied the method to a free fermion gas.

The relativistic free fermion theory

When we set all the link variables to the unit matrix in Eqs.(19) and (20), we get the free fermion theory. The random walks are set up in a very simple fashion. The moving point may step with probability 1/7 in each allowed direction. Back steps are forbidden by the properties of the Euclidean Dirac matrices.

Some importance sampling would be desirable in future applications, but we are not concerned with this important question here.

For the determination of S_{eff} we had to generate random walks which returned to the initial point. For each closed random walk we calculated the trace of the Dirac matrices along the loop. The calculation of the residues was done as described in section 4. We also note here that the stop probabili-

ties were automatically set to zero with our choice of the transition probabilities and we had to stop by fiat at the very end of the walks.

The calculation of M^{-1} proceeds in a similar fashion. There the random walks connect the two sites of the quark propagator. Otherwise the procedure remains the same as for the effective action.

If the random walks are implemented on an infinite lattice without boundary conditions, the coefficients C_{2n} of the hopping parameter expansion,

$$S_{eff} = \Sigma_n C_{2n} \cdot (\kappa^{2n}/2n), \qquad (21)$$

are determined by the method stochastically. The coefficients are also available from a deterministic calculation and a comparison is possible for the test of the method and the computer program.

The results of a test run are shown below. We initiated about a million random walks and the sucsessful ones were stored for later applications.

2n	C_{2n} (stochastic)	C_{2n} (exact)
4	$(9.58\pm0.12)\times10^{1}$	96
6	$(2.82\pm0.08)\times10^{3}$	2.82×10^{3}
8	$(8.30\pm0.36)\times10^{4}$	8.20×10^{4}
10	$(2.47\pm0.25)\times10^{6}$	2.46×10^{6}
12	$(7.99\pm0.65)\times10^{7}$	7.51×10^{7}
14	$(2.28\pm1.30)\times10^{9}$	2.30×10^{9}

We stopped by fiat after forty steps in the random walks of the above test run. The first fourteen powers of the expansion were very easy to generate with a modest amount of computer time. The higher terms require longer runs.

The effective action as a function of κ is shown in Fig.5.

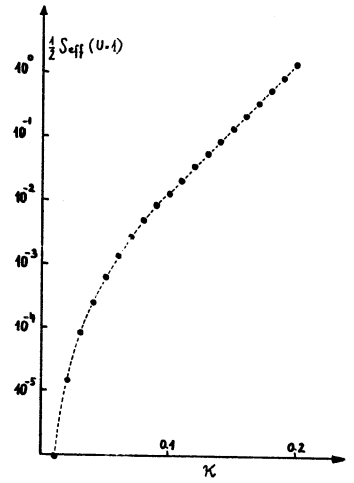

FIG.5. The effective action S_{eff} as a function of the hopping parameter κ including terms from the expansion up to the 14^{th} order. The dashed line represents the result of an exact calculation of S_{eff} on a large latticewith antiperiodic boundary condition.

We also made some test runs on lattices where the four dimensional lattice was infinite in the three spatial directions and finite in the imaginary time direction with antiperiodic boundary condition for the quarks. This configuration corresponds to the thermodynamics of the free relativistic quark gas of vanishing chemical potential. The temperature of the system is given by the inverse size of the lattice in the fourth direction. The free energy of the relativistic free quark gas at vanishing chemical potential is calculable from the finite size dependence of the partition function. S_{eff} is depicted in Fig.6 as the function of the inverse temperature N_β in dimensionless units.

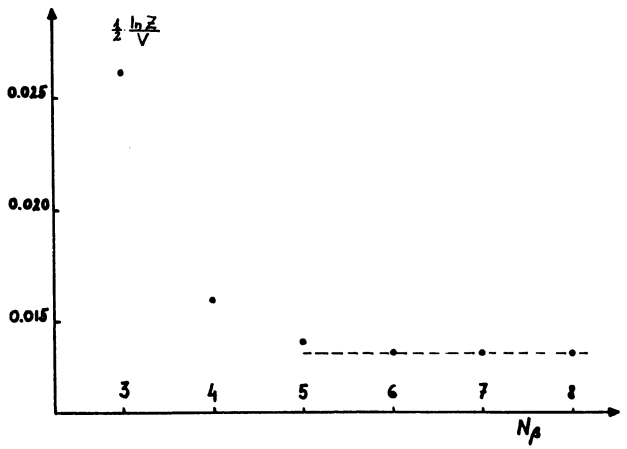

FIG.6. The logarithm of the partition function divided by the four-dimensional volume V is depicted for the relativistic free fermion gas as a function of the inverse temperature N_β for various lattice sizes in the fourth direction. The curve is shown for $\kappa = 0.1$.

Quark vacuum polarization in QCD

We return now to the full QCD problem in our stochastic treatment of the quark vacuum polarization. The procedure remains the same as in the free fermion case, but the algorithm becomes more involved.

We apply the standard Metropolis procedure to the updates of the gauge link variables. The algorithm and the corresponding computer program are organized in the following fashion.

At the beginning of the calculation we generate closed loops for the later evaluation of the effective action in the above described manner. The loops are stored on disc together with their characteristic parameters. This procedure can be repeated from time to time during long runs of the code.

During the updating step we randomly select a subset of the generated loops and use them in the decision making procedure when the change in S_{eff} has to be calculated. For the calculation of the quark propagator the method is applied again to M^{-1}.

In our first test runs only a few limited applications were tried so far. Since the program is not implemented yet on the GSI array processor, we strongly limited the length of the closed loops in the calculation of δS_{eff}.

In order to make the thermodynamical applications more efficient and more reliable, the thermal Wilson loop[15], which wraps around the fourth direction, was built into the action directly.

We also made some test runs in the quenched approximation. Fig.7 shows the mean value of the effective action in the quenched approximation when the system is updated with respect to S_0 only. The free theory is indicated by the solid line. The points are shown for various values of the coupling constant β.

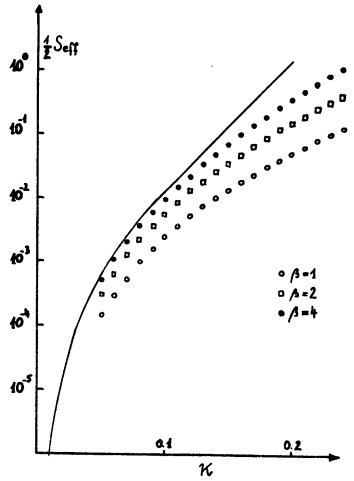

FIG.7. The mean value of the effective action is shown here in the quenched approximation.

As a final step in the program development, the full updating procedure including the fermion vacuum polarization in S_{eff} was implemented. First we calculated the thermal Wilson loop in the presence of quark vacuum polarization. Some results are given in Fig.8.

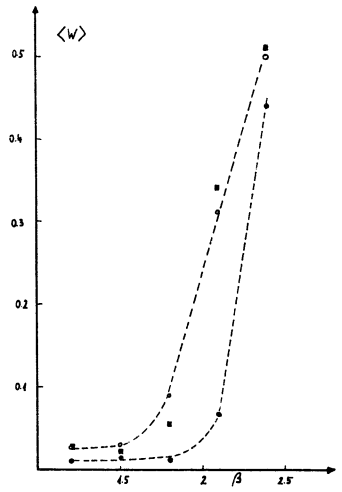

FIG.8. The thermal Wilson loop as a function of the coupling is shown here on a lattice of dimension $6^3 x 3$. The full dots correspond to runs where the quark vacuum polarization was switched off from the updating procedure. The open circles indicate points from runs where in addition to S_0 the thermal loop itself was included directly into the effective action. The squares were obtained from runs in which the quark vacuum polarization was fully implemented in the Metropolis procedure.

Though the first test runs were limited to relatively short loops in the effective action, the results are interesting. The abrupt change in the thermal Wilson loop is still there as in the pure gauge sector, though the location is shifted toward stronger couplings. That presumably indicates that the phase transition into quark-gluon matter occurs at lower physical temperature than in the pure gauge sector.

We will return to a more detailed description of our algorithm in the near future[16]. Presumably, we will have better results on larger lattices and longer random walks at that later time.

Finally, we want to mention that also some other stochastic methods were recently proposed[17] for the fermion problem in QCD.

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